Multiscale PIC modeling of beams and plasmas.

J.-L. Vay
Heavy Ion Fusion-Virtual National Lab./Lawrence Berkeley National Lab.

In collaboration with:

- **A. Friedman, D.P. Grote, R.H. Cohen - HIF-VNL/Lawrence Livermore Nat. Lab.**
- **P. Colella, McCorquodale, D. Serafini - Lawrence Berkeley Nat. Lab.**
- **J.-C. Adam, A. Héron - CPHT, Ecole Polytechnique, France**
- **E. Sonnendrücker, Université de Strasbourg, France**

Ecole CEA-EDF-INRIA / *CEA-EDF-INRIA School*
Kinetic equations. Applications to plasma and beam physics.
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Outline

- Who we are. Our interest in multiscale modeling.
- Modeling of plasmas: generalities.
- AMR
  - issues
  - Electrostatic
    - modeling of the High-Current Experiment (HCX)
    - modeling of the Large Hadron Collider (LHC)
  - Electromagnetic
    - modeling of laser-plasma interaction
  - Vlasov
- New particle mover for large time steps in magnetic fields
- Toward multiscale modeling of plasmas: some methods
- Conclusion

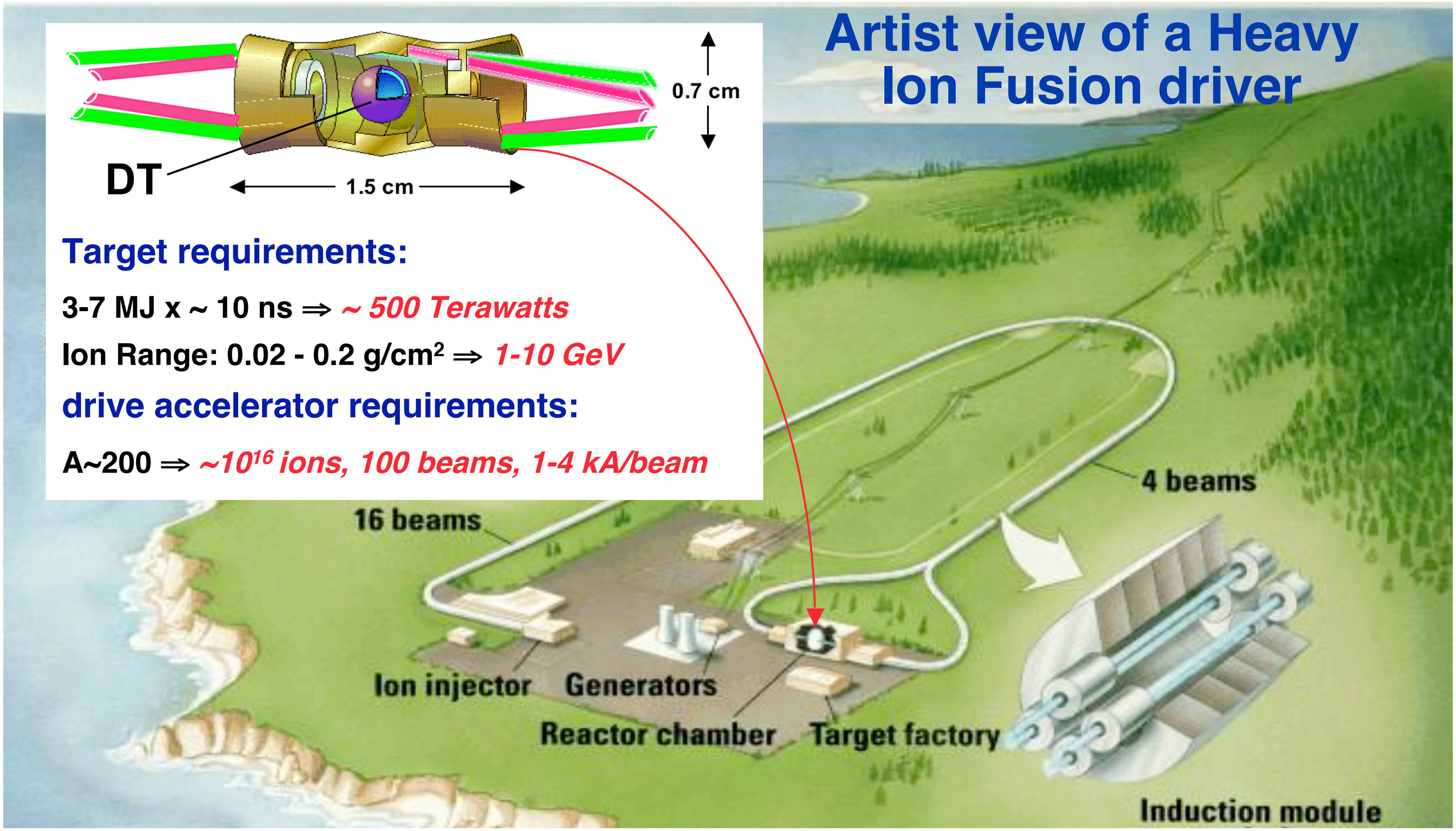
The U.S. Heavy Ion Fusion Program - Participation

Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Princeton Plasma Physics Laboratory
Naval Research Laboratory
Los Alamos National Laboratory
Sandia National Laboratory
University of Maryland
University of Missouri
Stanford Linear Accelerator Center
Advanced Magnet Laboratory
Idaho National Environmental and Engineering Lab
University of California
  a. Berkeley
  b. Los Angeles
  c. San Diego

MIT
Advanced Ceramics
Allied Signal
National Arnold
Hitachi
Mission Research
Georgia Tech
General Atomic
MRTI

Employees of LBNL, LLNL, and PPPL form the U.S. Virtual National Laboratory for Heavy Ion Fusion

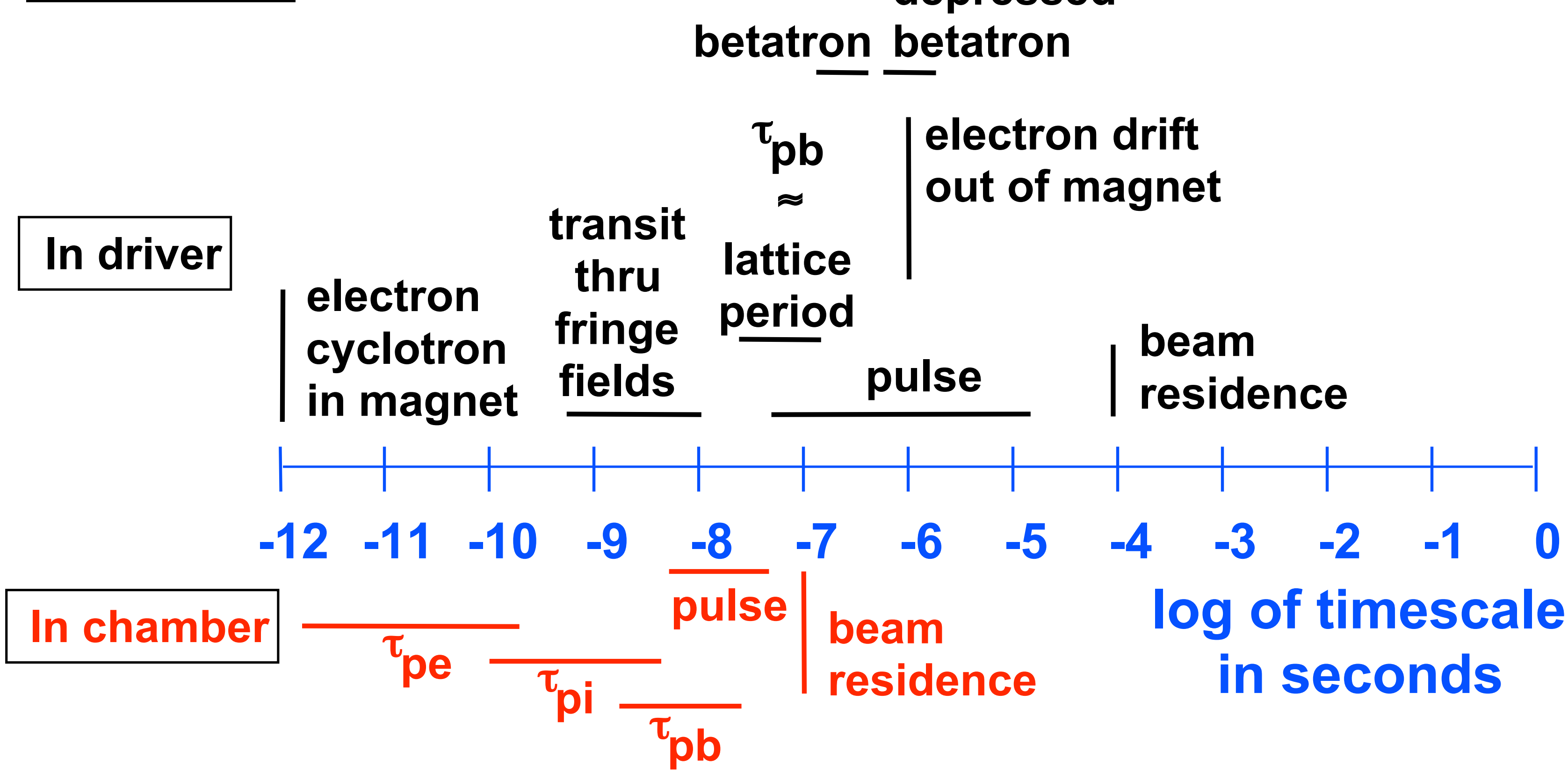
Heavy Ion Inertial Fusion (HIF) goal is to develop an accelerator that can deliver beams to ignite an inertial fusion target



How near term goal is High-Energy Density Physics (HEDP).

Time and length scales in driver and chamber span a wide range

Time scales:



Length scales:

- electron gyroradius in magnet ~10 μm
- $\lambda_{D,beam}$ ~ 1 mm
- beam radius ~ cm
- machine length ~ km's

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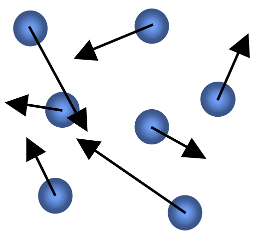
Modeling of a plasmas - classification (1)

- Collection of a large number of interacting charged particles
  - Particles mathematically described by
    - Lagrangian approach: evolution of singularities
      - Klimontovitch eq.
    - Eulerian approach: evolution of an incompressible fluid
      - in phase-space: Boltzmann/Fokker-Planck eq. (collisions), Vlasov eq. (no collisions)
      - in real space: fluid/MHD eq.
  - Interactions mathematically described by
    - Lagrangian approach: sum from all singularities, instantaneous or with retardation
    - Eulerian approach: fields
      - instantaneous: Poisson
      - with retardation: Maxwell

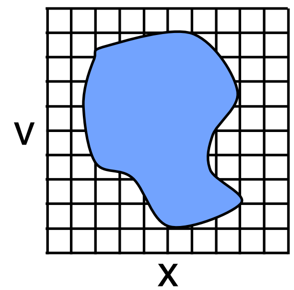
Modeling of a plasmas - classification (2)

- **In summary, the modeling of a plasma implies the modeling of**

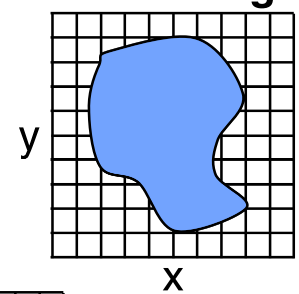
a collection of particles **fluid cells in phase-space** **fluid cells in configuration space**



or

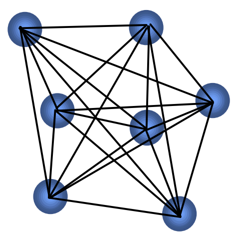


or

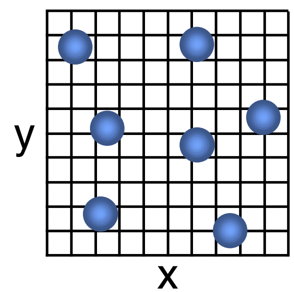


interacting

directly



or through a field



- **The numerical integration leads to further splitting**
  – **Partial differential equations: finite-differences/volumes/elements, Monte-Carlo, semi-Lagrangian,**
  – **Time integration: explicit/implicit,**
  – **Direct interaction: direct summation, multipole expansion (tree-codes),**
  – **…**

Modeling of a plasmas - commonalities, speed-up

- All these methods have in common that they must update the status of N quantities (particle/fluid/field quantities) from time t to time t+Δt
- In order to minimize the computing time, N/Δt should be minimized
  - grids: non-uniform, block-structured, high-order splines, filtering,
  - time steps: non-uniform, different for particle groups (species, velocity, …), different for grid blocks (with different Δx), high-order integrators, averaging over smallest time scales,
  - particles: splitting/merging, high-order splines, filtering,
  - hybrids

    - Groups of particles modeled differently, according to species, velocities, momentum, charge state, …

    - particle-particle-particle-mesh (pp-pm),

    - regions modeled differently (for example implicit in high-density parts, explicit in low-density parts)
  - …
- The subject is very large. We will focus on a few recent developments.

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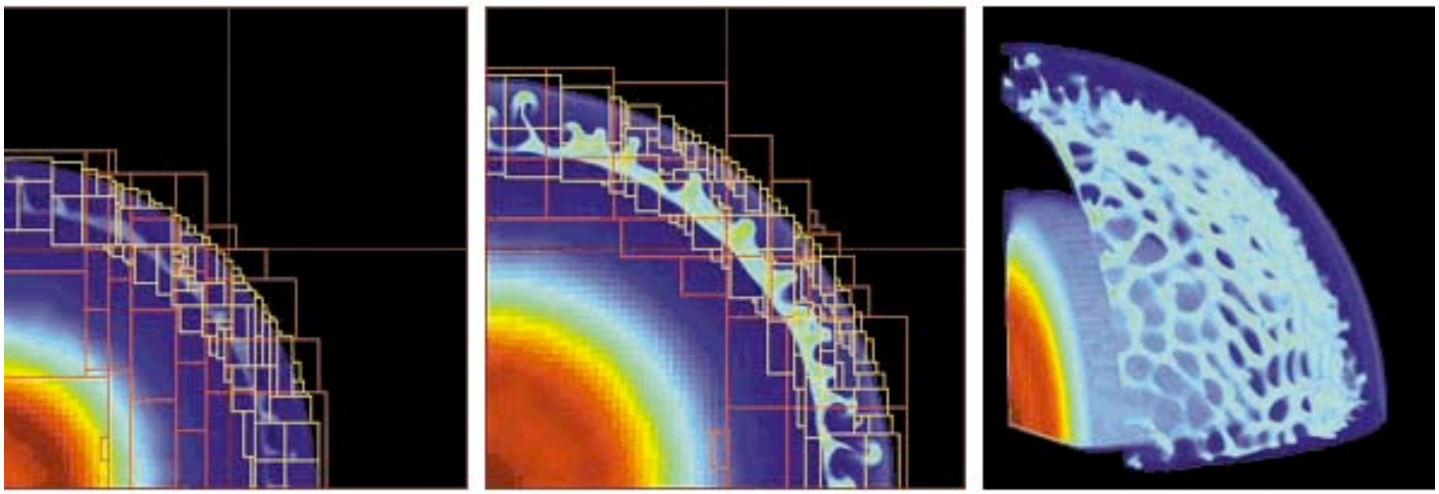
The Adaptive-Mesh-Refinement (AMR) method

- **addresses the issue of wide range of space scales**
- **well established method in fluid calculations**

3D AMR simulation of an explosion (microseconds after ignition)



AMR concentrates the resolution around the edge which contains the most interesting scientific features.

- **however, coupling to PIC/Vlasov/MHD methods has to be done with care**

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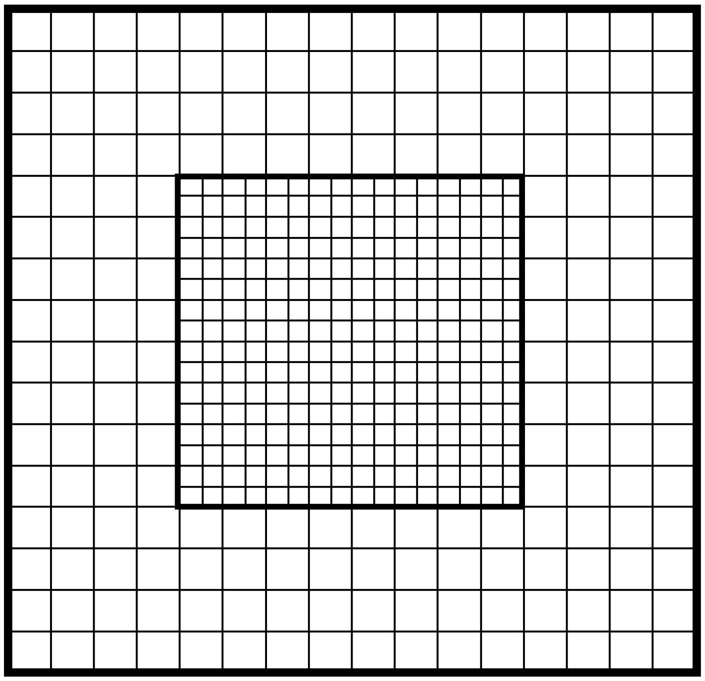
Coupling of AMR to PIC/Vlasov/MHD: issues

Mesh refinement implies a jump of resolution and some procedure for coupling the solutions at the interface. What kind of issues can we expect?



- loss of symmetry: self-force?

- conservation laws?

- waves (EM, plasma)?

We will look at some of these aspects using simple schemes in reduced dimensions.

Example: 2-D PIC-electrostatic

- Given a hierarchy of grids, there exists several ways to solve Poisson.

- Two considered here:

1. '1-pass'
- solve on coarse grid
- interpolate solution on fine grid boundary
- solve on fine grid
- ➢ different values on collocated nodes

2. 'N-pass'
- interleave coarse and fine grid relaxations
- collocated nodes values reconciliation
- ➢ same values on collocated nodes

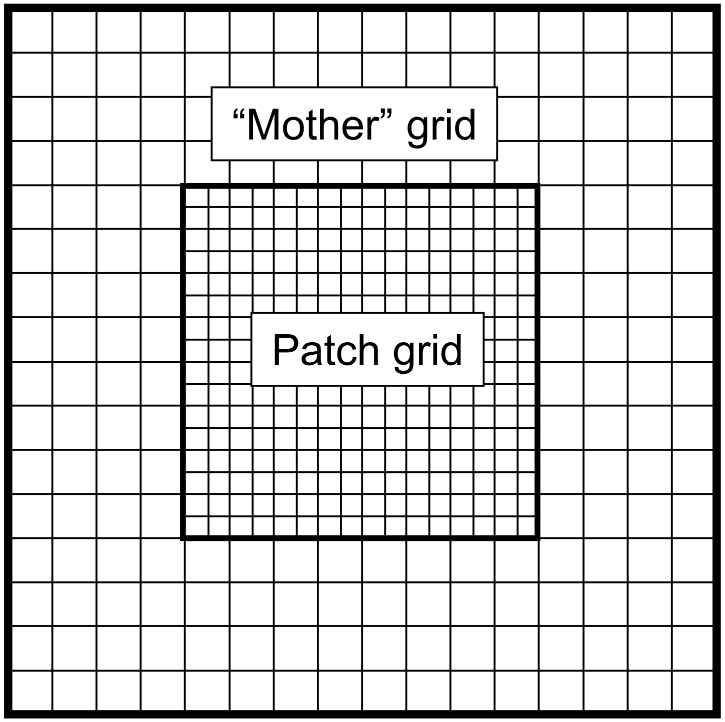
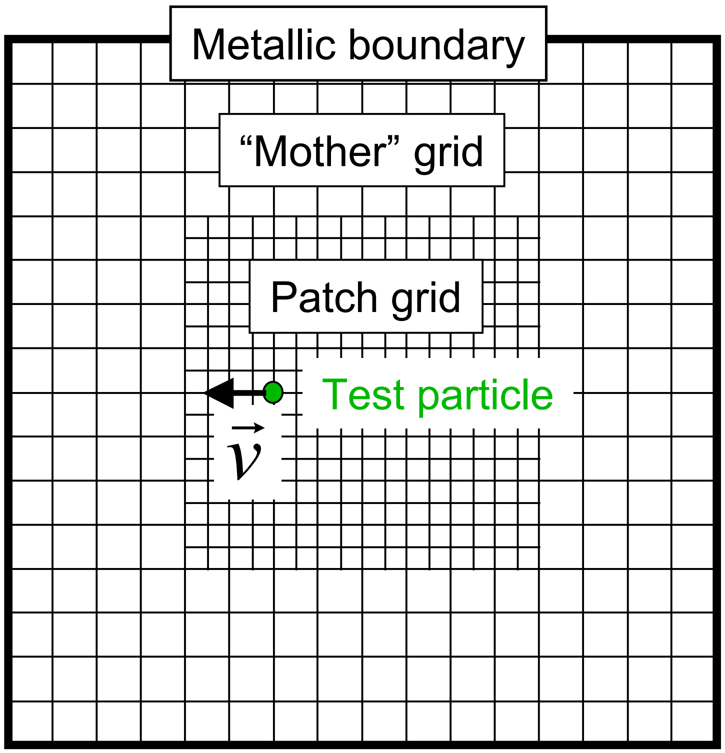
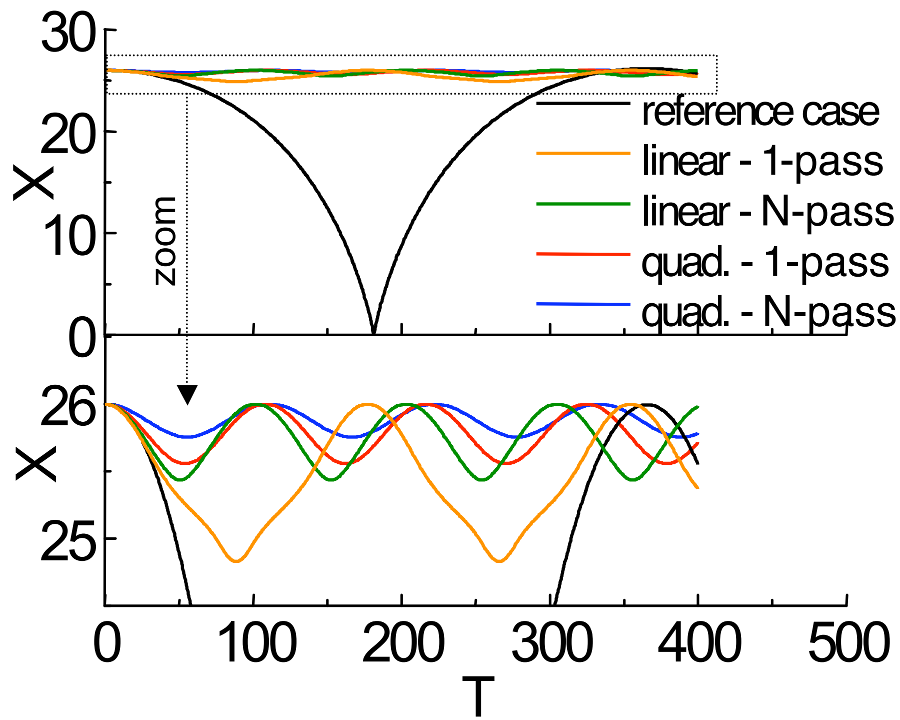


Illustration of the spurious self-force effect

- 1 grid with metallic boundary + 1 refinement patch



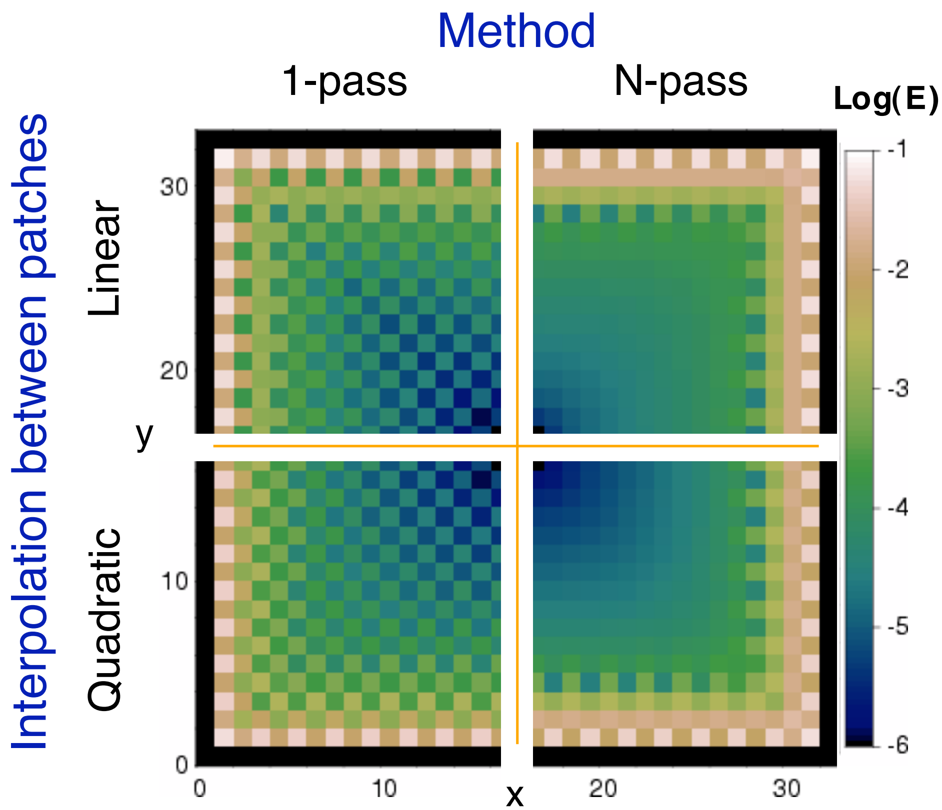
one particle attracted by its image

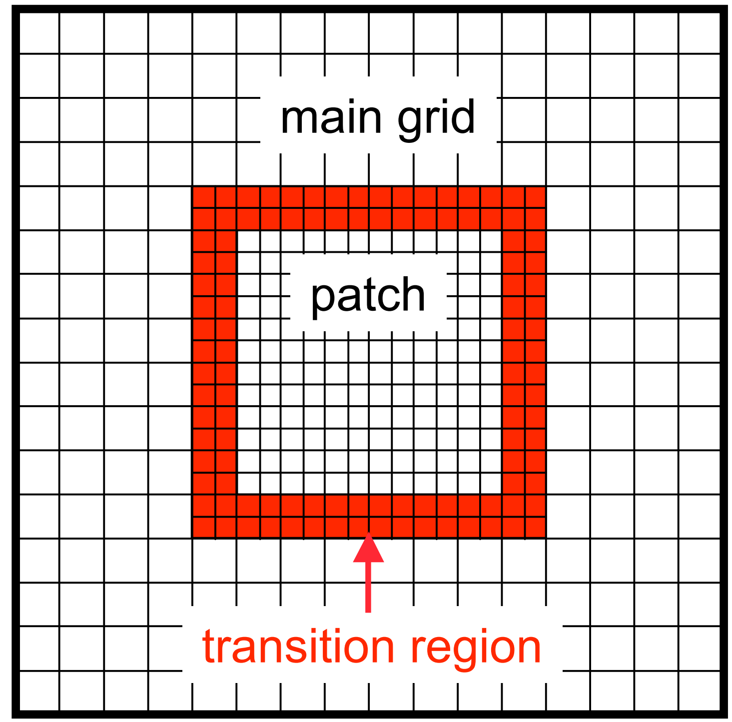


particle trapped in patch

$\Rightarrow$ MR introduces spurious force,

Self-force amplitude map and mitigation

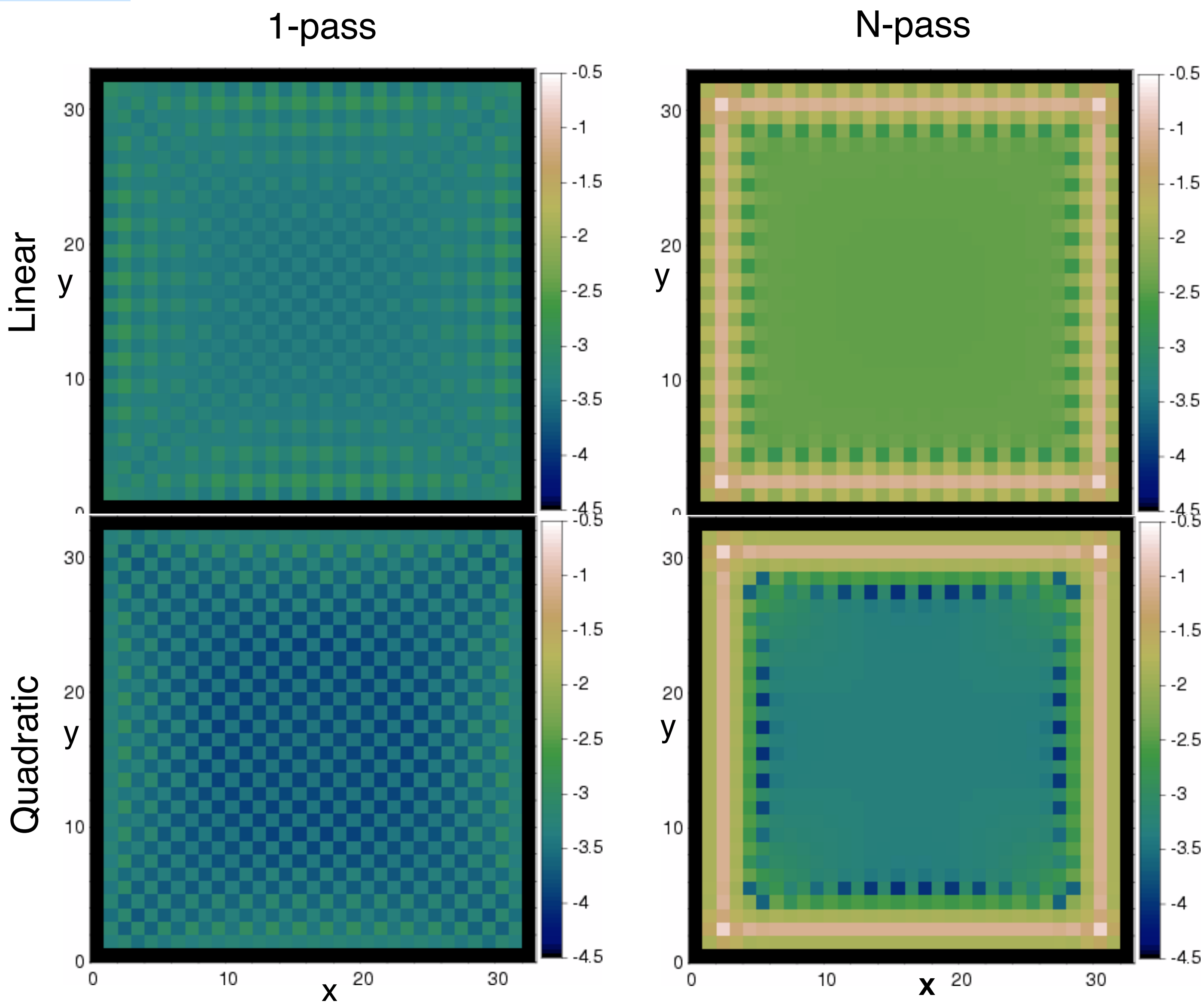




- Magnitude of self force decreases rapidly with distance from edge
- with the 1-pass method, the coarse grid solution is free of self-force:
  - ⇒ the self-force effect can be mitigated by defining a transition region surrounding the patch in which deposit charge and solve, but get field from underlying coarse patch
- N-pass method: coarse grid solution has spurious self-force
  - ⇒ no easy mitigation method

Global error

$$\sum \left| (\phi - \phi_{ref}) / \phi_{ref} \right| / N$$



⇒ global error larger with N-pass than 1-pass

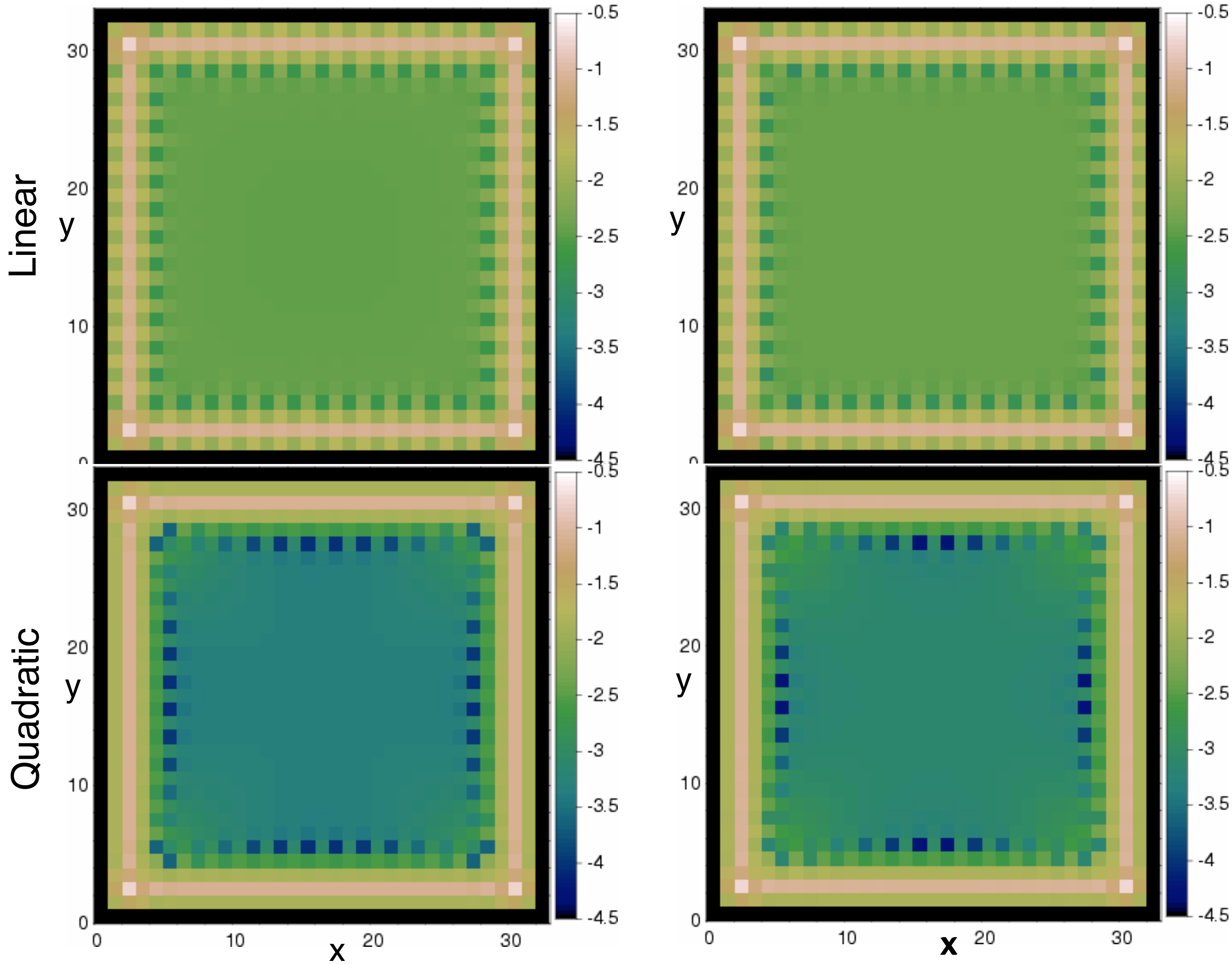
Global error

$$\sum \left| \left(\phi - \phi_{ref} \right) / \phi_{ref} \right| / N$$

N-pass

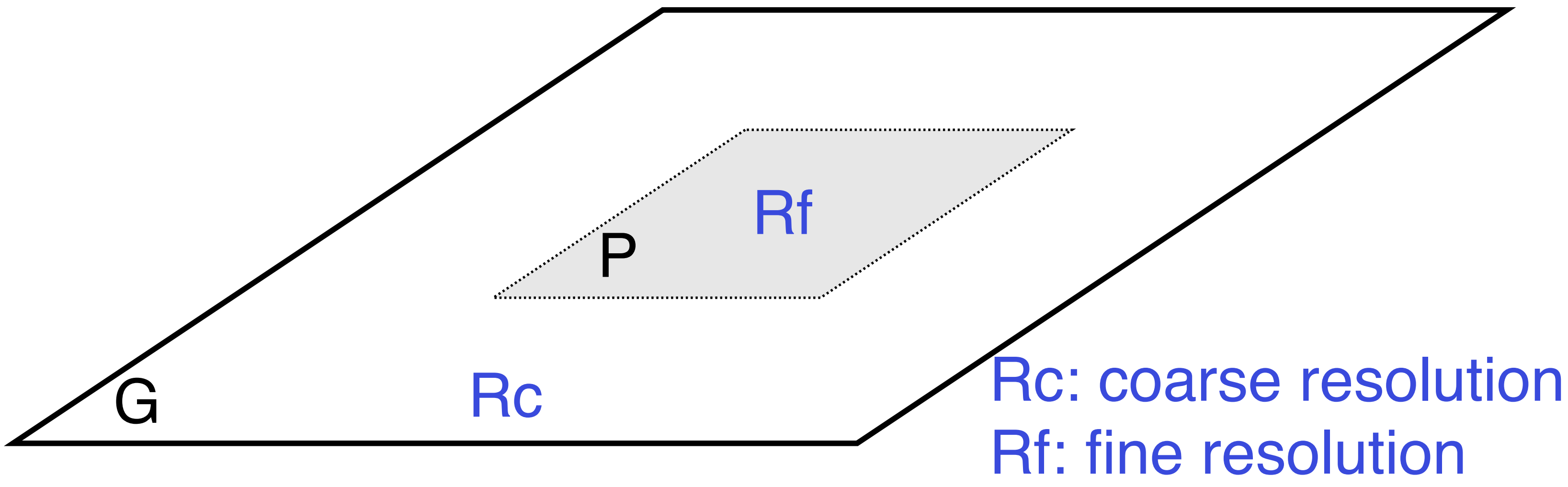
$$\left| \oiint_S \vec{D} \cdot \vec{d}S - \iiint_V \rho d\tau \right| / \iiint_V \rho d\tau$$

N-pass



⇒ N-pass: global error due to violation of Gauss' law

Electromagnetics: usual scheme



• the solution is computed as usual in the main grid and in the patch

• interpolation is performed at the interface

1-D AMR-EM

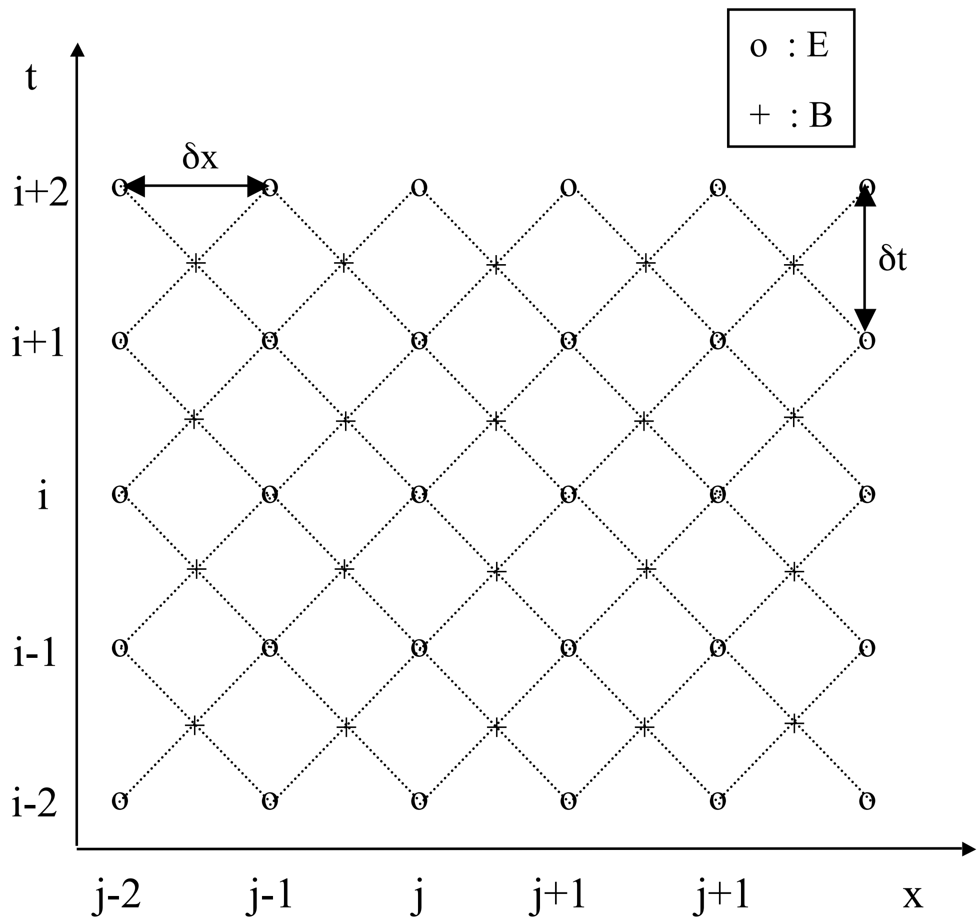
- **We consider 1d wave equation**

$$\frac{\partial E}{\partial t} = \frac{\partial B}{\partial x}; \quad \frac{\partial B}{\partial t} = \frac{\partial E}{\partial x}$$

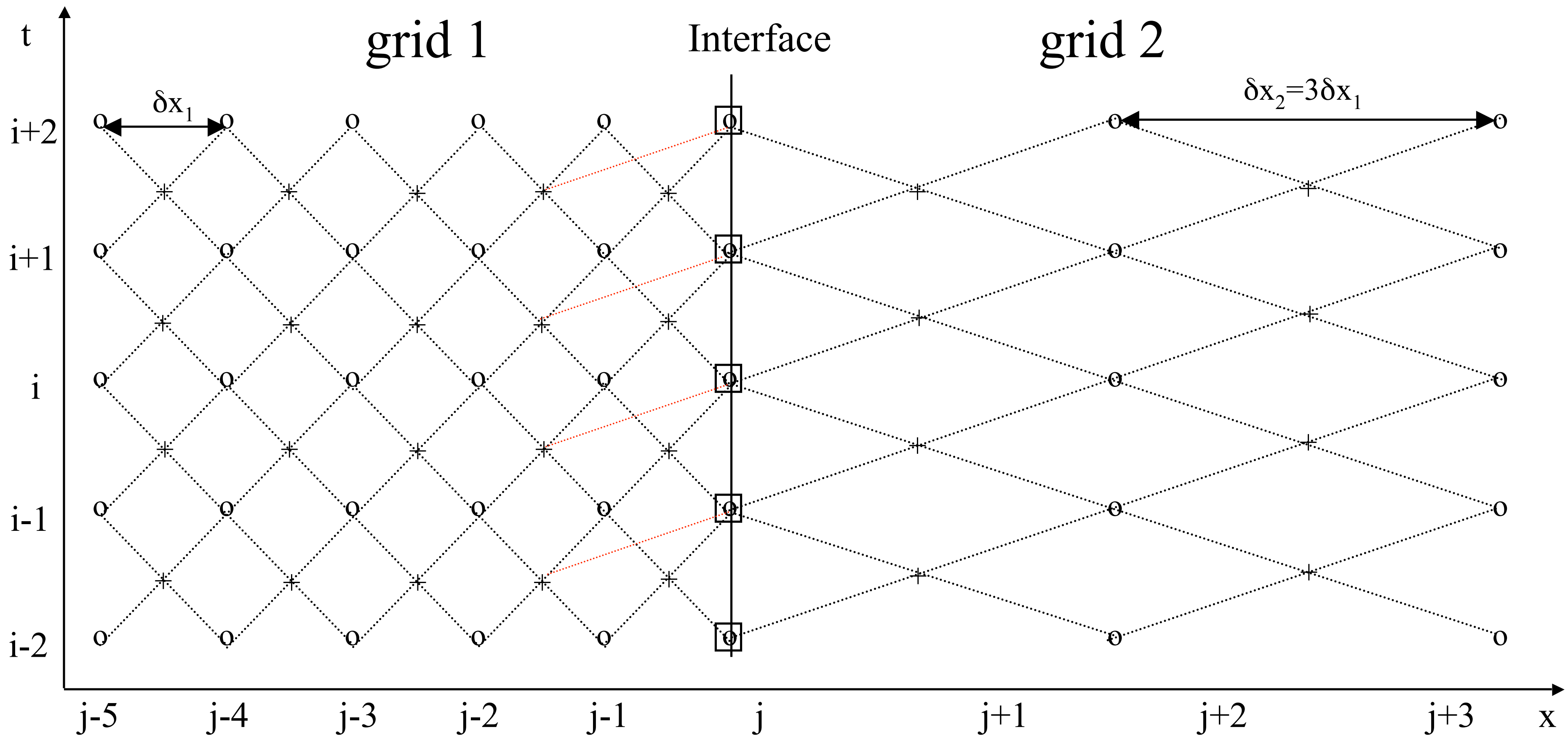
- **staggered on a regular space time grid**
- **We use finite-difference time-centered scheme**

$$\frac{E_j^{i+1} - E_j^i}{\delta t} = \frac{B_{j+1/2}^{i+1/2} - B_{j-1/2}^{i+1/2}}{\delta x}$$

$$\frac{B_{j+1/2}^{i+1/2} - B_{j+1/2}^{i-1/2}}{\delta t} = \frac{E_{j+1}^i - E_j^i}{\delta x}$$



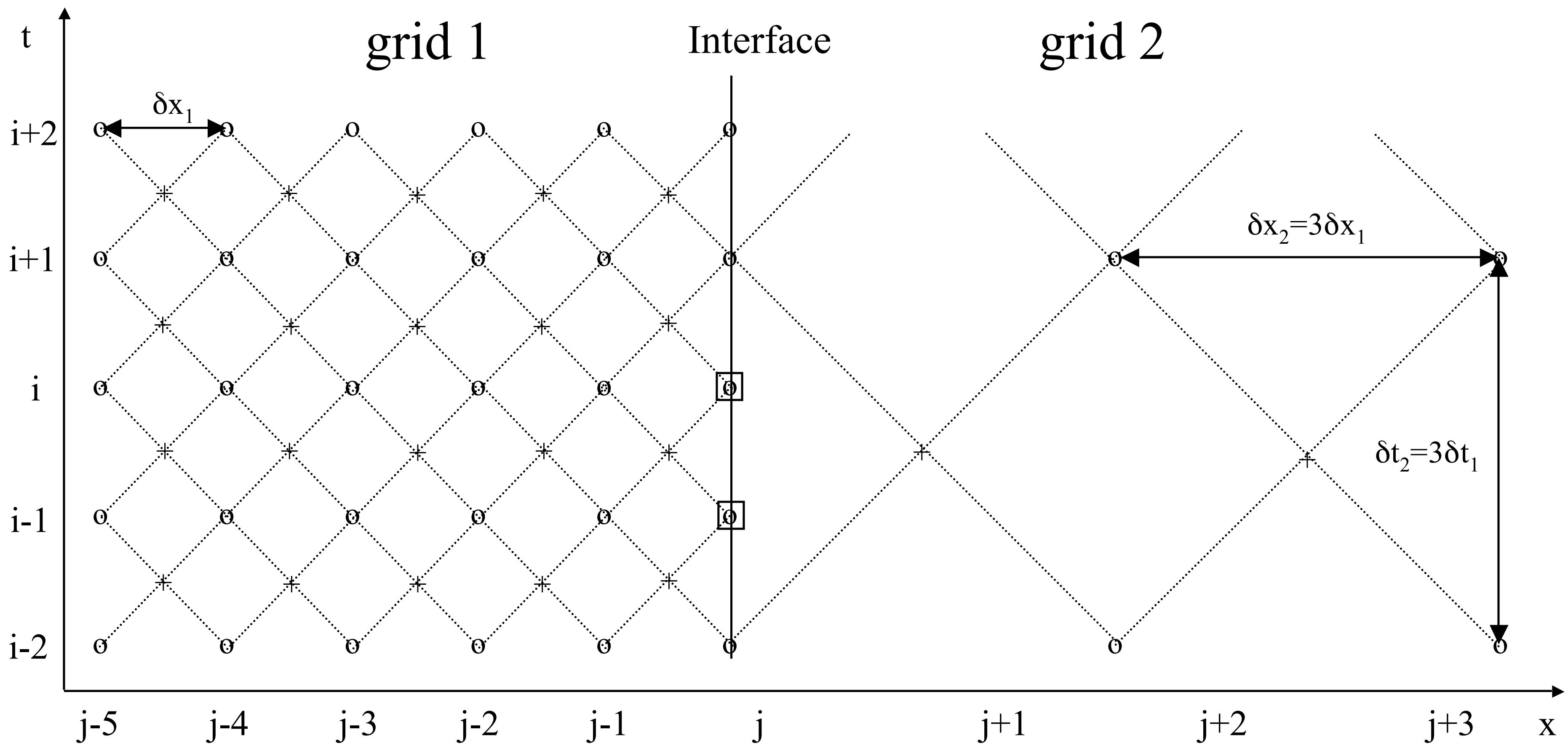
1-D AMR-EM: space refinement only (factor 3)



o, + : finite-difference

o : finite-volume or 'jump' inside fine grid

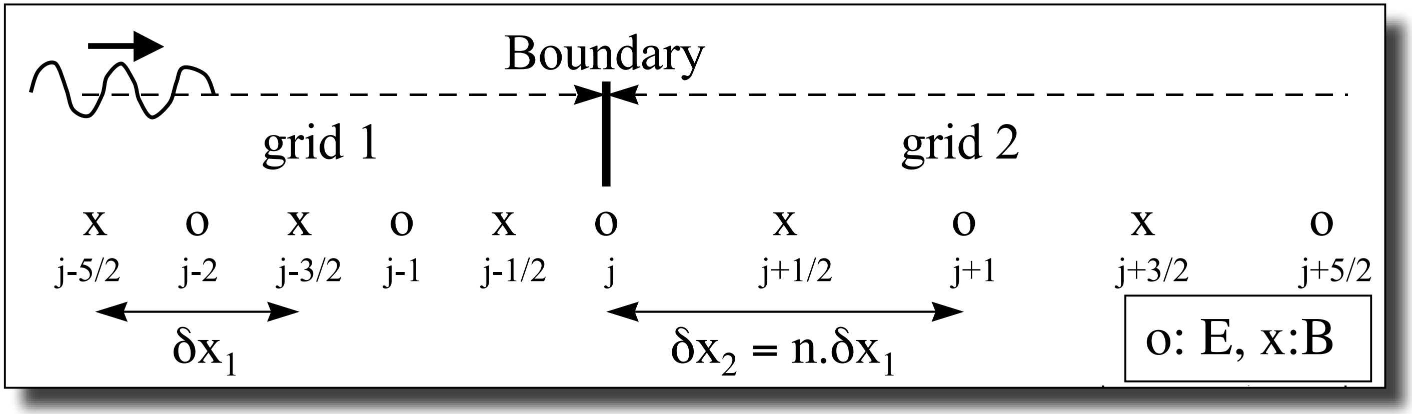
1-D AMR-EM: space and time (factor 3)

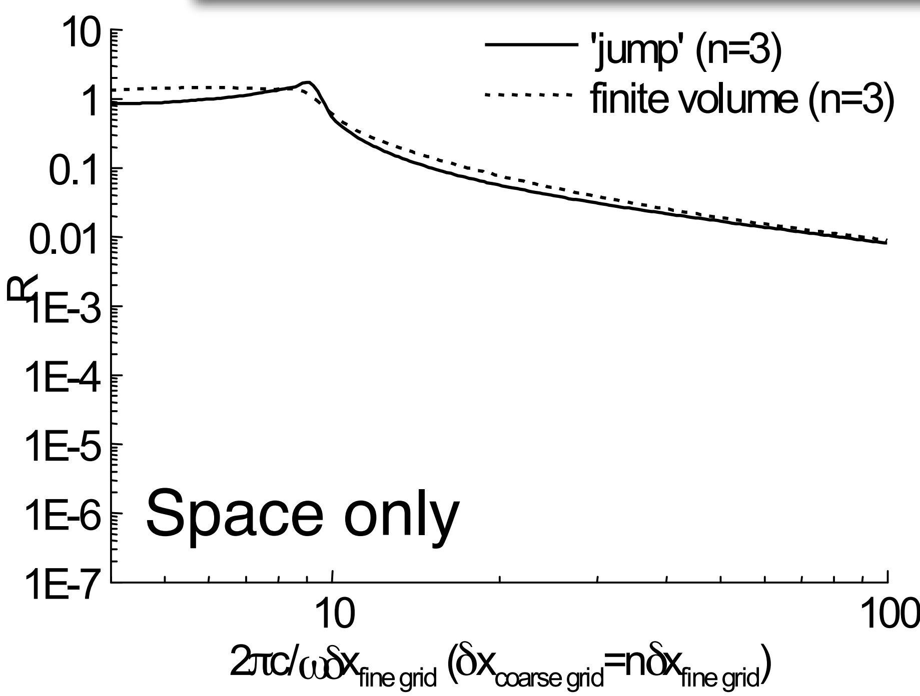


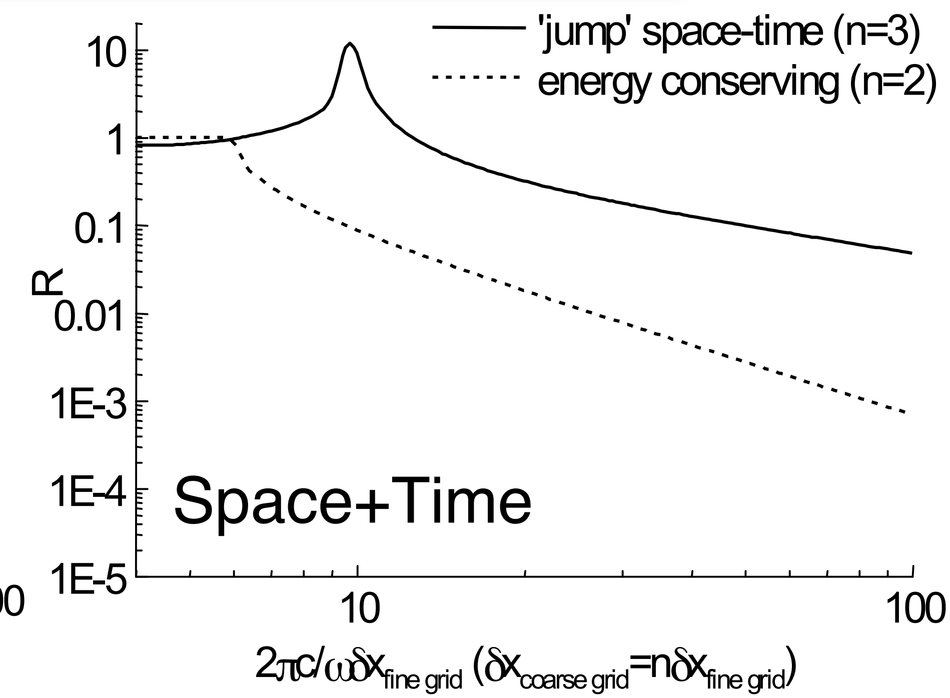
o, + : finite-difference

$\boxed{o}$: interpolated from previous and next computed values

1-D AMR-EM: illustration of instability*

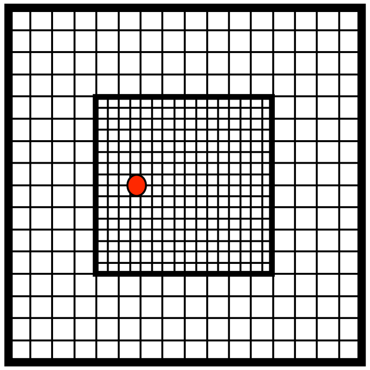






* J.-L. Vay, JCP (2001)

Coupling of AMR to PIC/Vlasov/MHD: Issues (summary)



1. Asymmetry of grid implies asymmetry of field solution for one particle/marker/fluid cell
   - spurious self-force

2. Some implementations may violate Gauss' Law
   - total charge may not be conserved exactly

3. EM: shortest wavelength resolved on fine grid not resolved on coarse grid may reflect at interface
   - if reflection factor <=1, spurious waves
   - if reflection factor >1, may cause instability by multiple reflections

Remark: BTW, these are general and apply also to irregular griddings!

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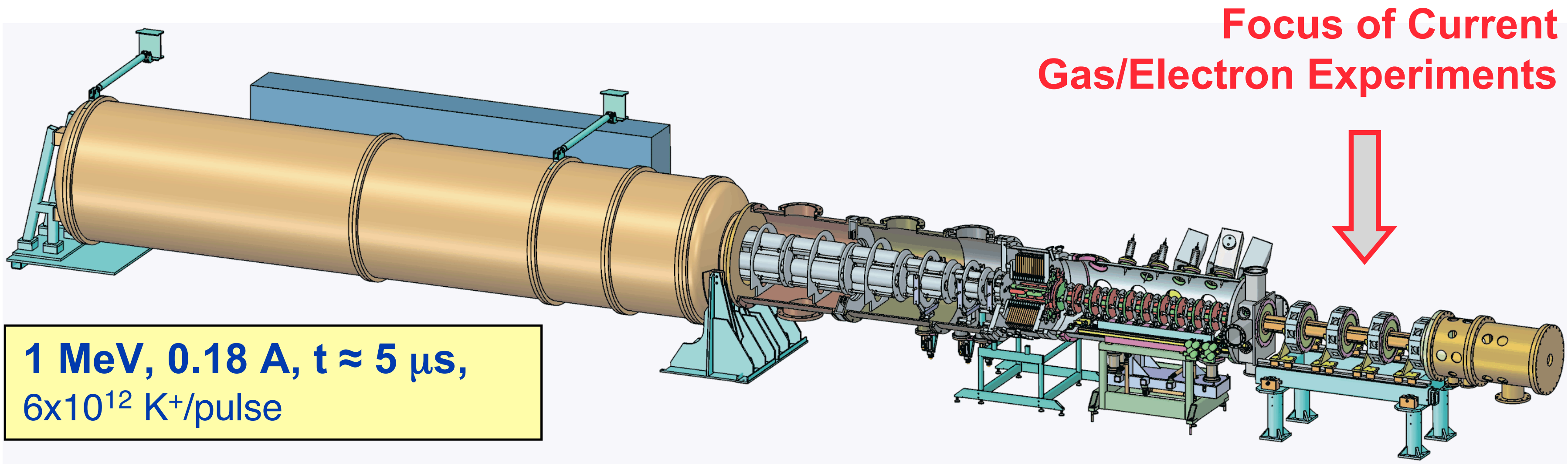
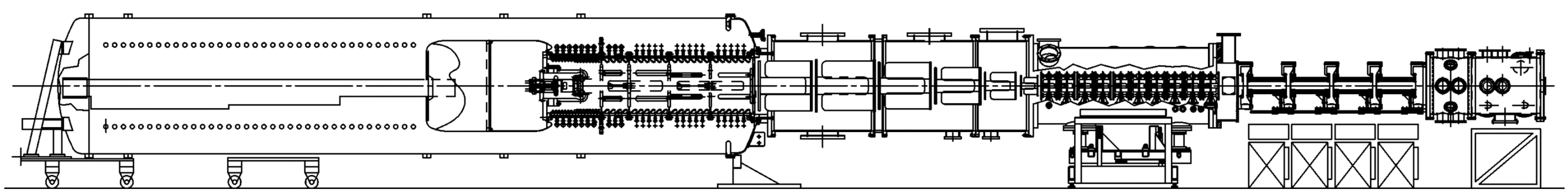
Current HCX Configuration
(High Brightness Beam Transport Campaign, 2005)





<u>Additional Experiments:</u> Fill-Factor Measurements, Head-Tail Correction, Wave Experiments

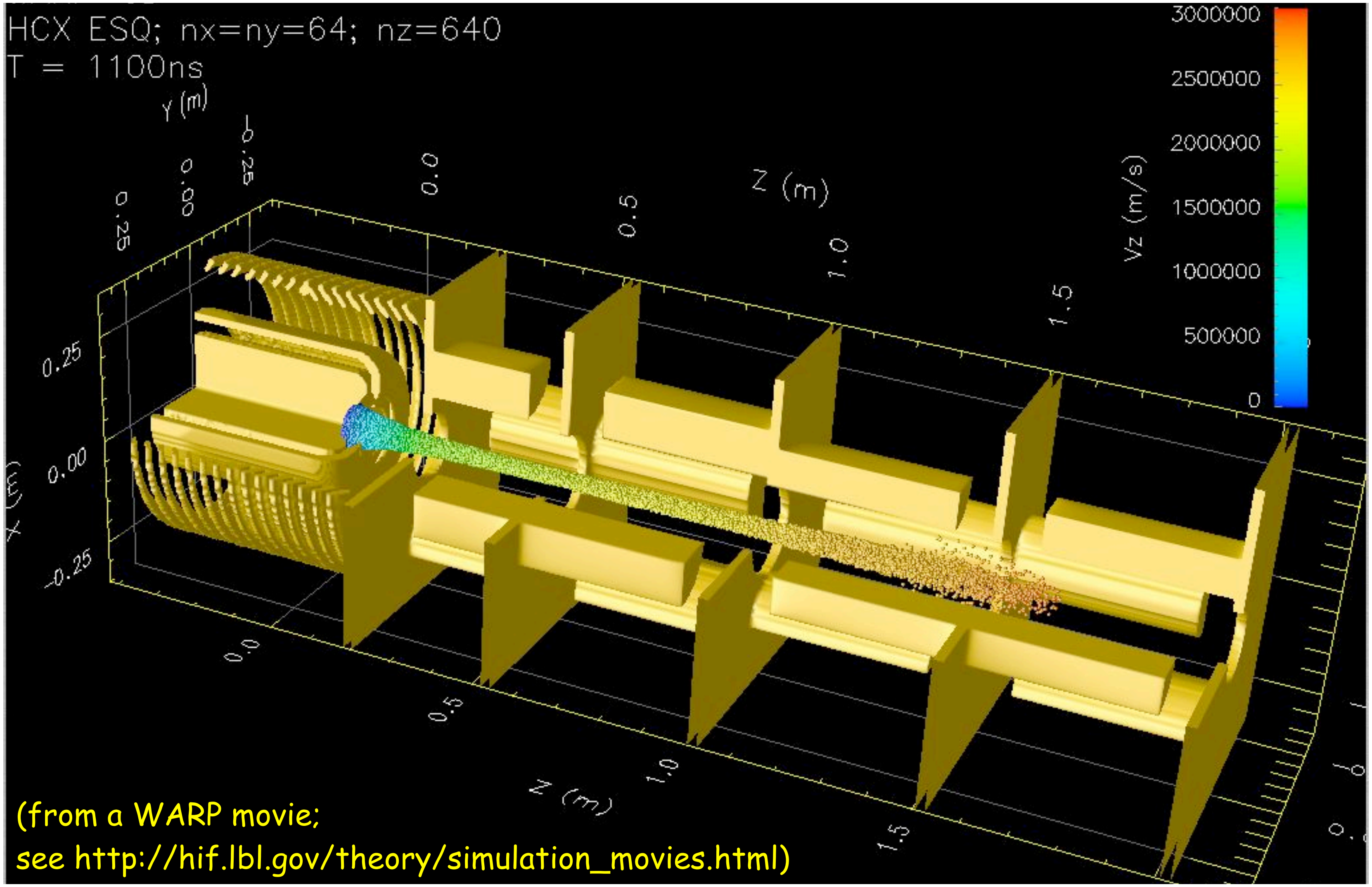
We are using the accelerator PIC code WARP.

- **Geometry:** 3D, (x,y), or (r,z)
- **Field solvers:** FFT, capacity matrix, multigrid
- **Particle pusher:** Boris, subcycling
- **Boundaries:** "cut-cell" --- no restriction to "Legos"
- **Bends:** "warped" coordinates; no "reference orbit"
- **Lattice description:** general; takes MAD input
  - solenoids, dipoles, quads, sextupoles, …
  - arbitrary fields, acceleration
- **Beam injection:** Child-Langmuir, and other models
- **Diagnostics:** Extensive snapshots and histories
- **Parallel:** MPI
- **Python and Fortran:** "steerable," input decks are programs
  - a GUI is also available

New advanced features:

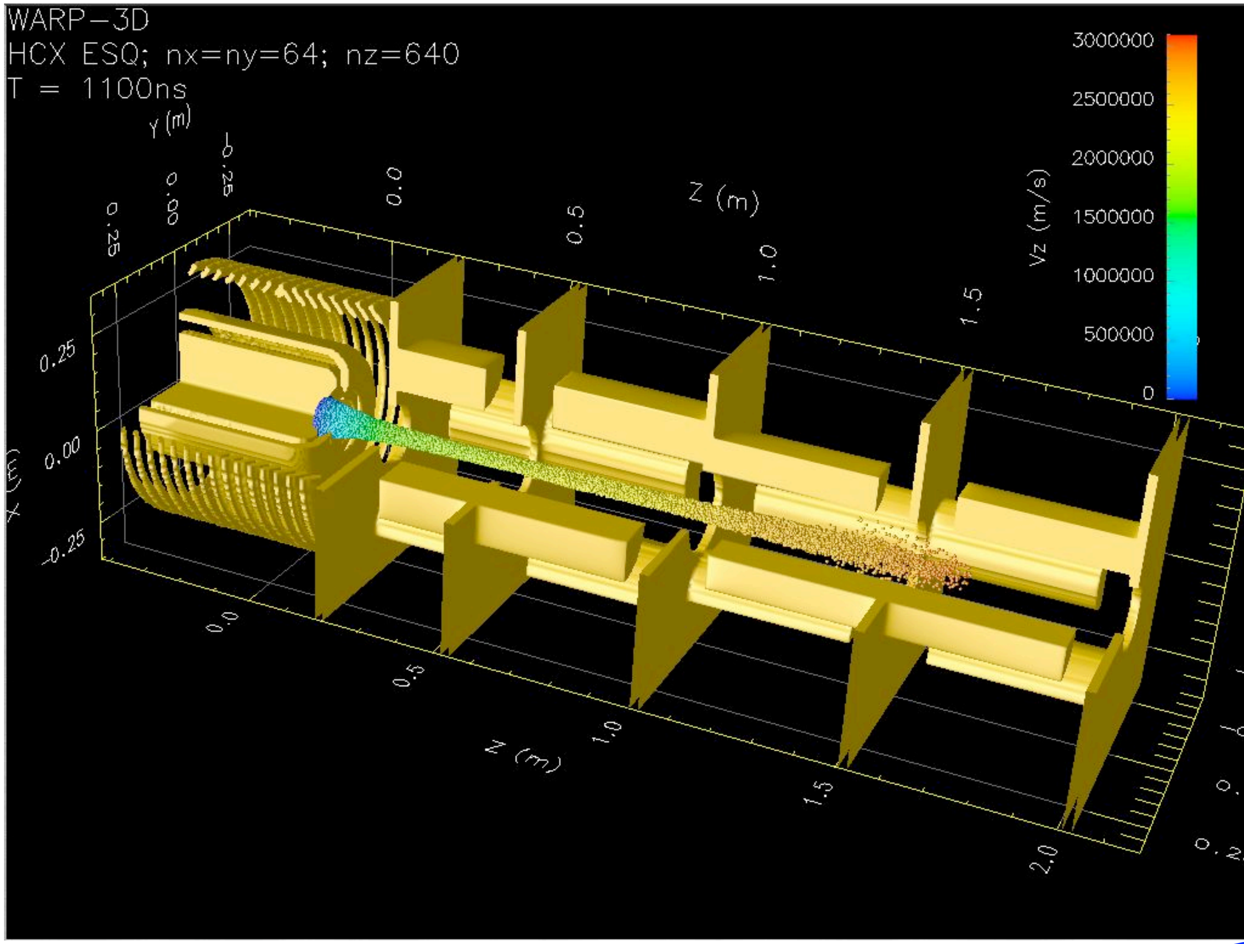
- AMR, Electron mover with large time steps, gas and electrons models, prototype Vlasov (soon)

3-D WARP simulation of High-Current Experiment (HCX)

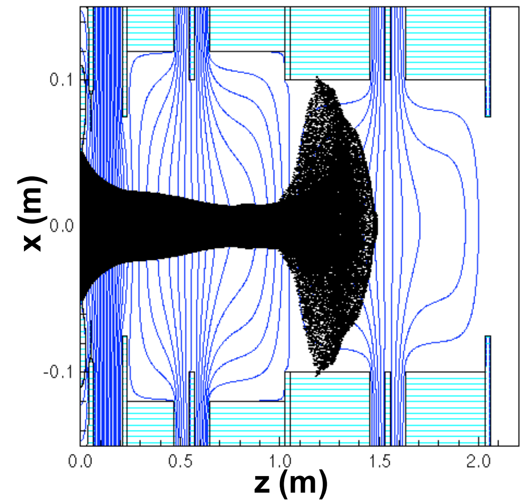


In the following slides, we will follow the story of the why and how we implemented mesh refinement to get to numerical convergence.

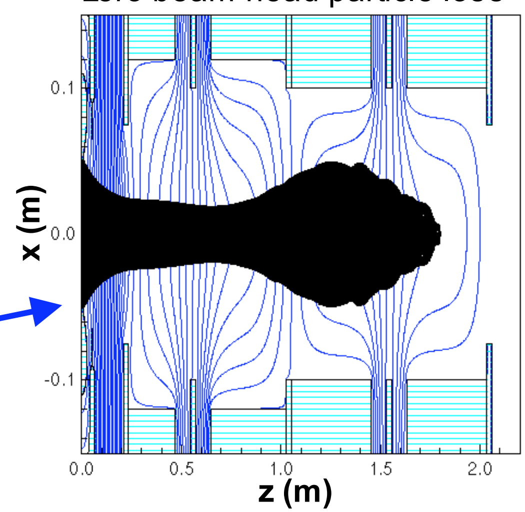
3-D WARP simulation of HCX shows beam head scrapping



Rise-time τ = 800 ns
beam head particle loss < 0.1%

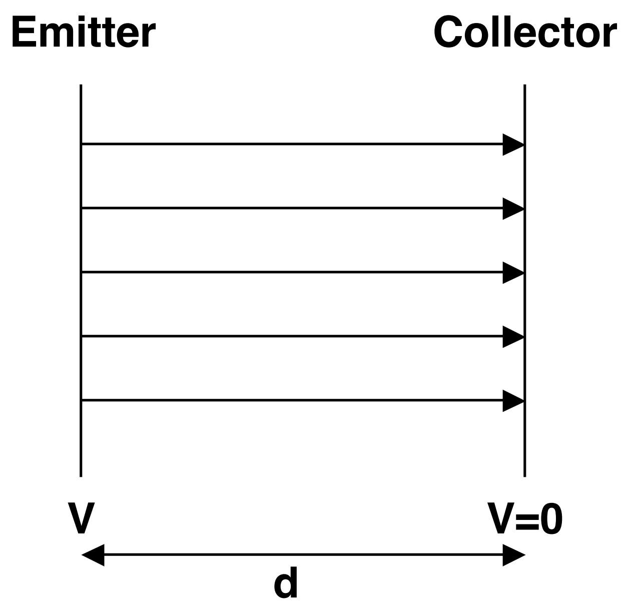


Rise-time τ = 400 ns
zero beam head particle loss

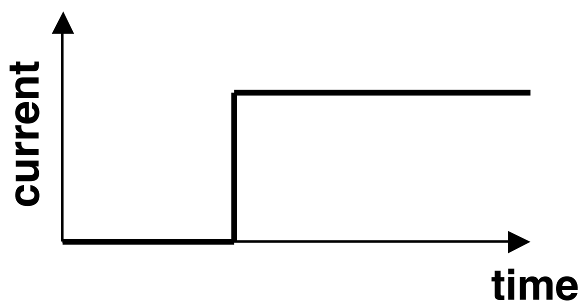


- **Head cleaner with shorter voltage rise-time.**
- **Questions:**
  - **what is the optimal rise-time?**
  - **can we produce and model very-fast rise-time?**

Test: 1-D time-dependent modeling of ion diode



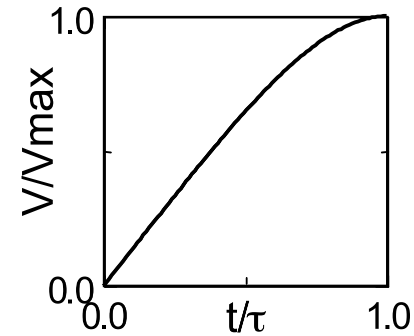
Applied voltage for Heavyside current history?

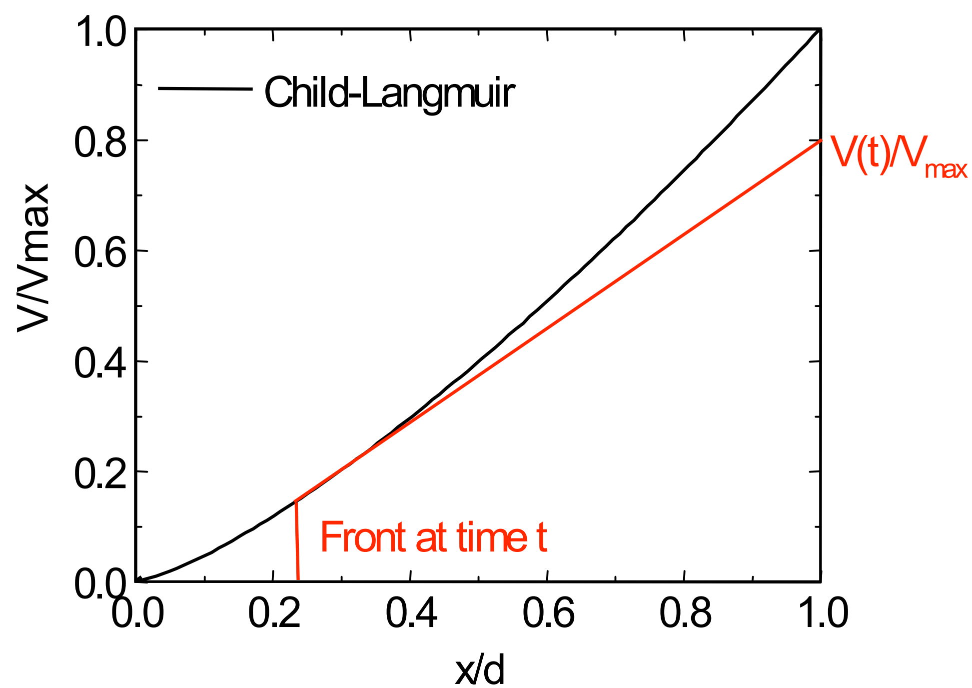


Analytic solution from Lampel-Tiefenback

$$V(t) = \frac{t}{3\tau}\left[4 - \left(\frac{t}{\tau}\right)^3\right]V_{\max}$$

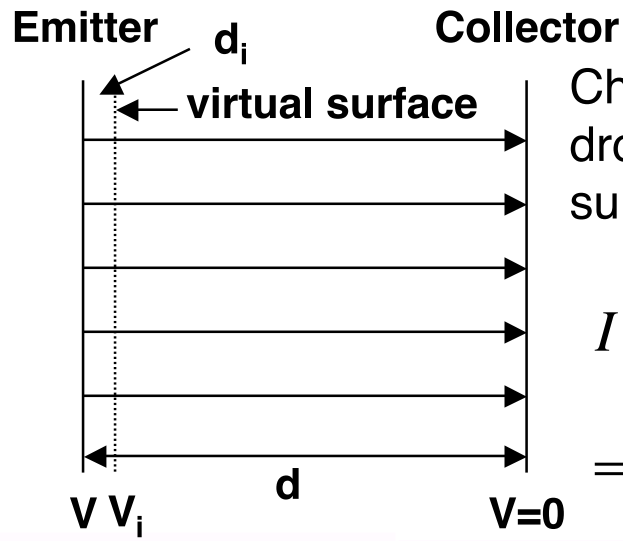
(τ: transit time)





Test: 1D time-dependent modeling of ion diode (algo 1)

Injection algorithm

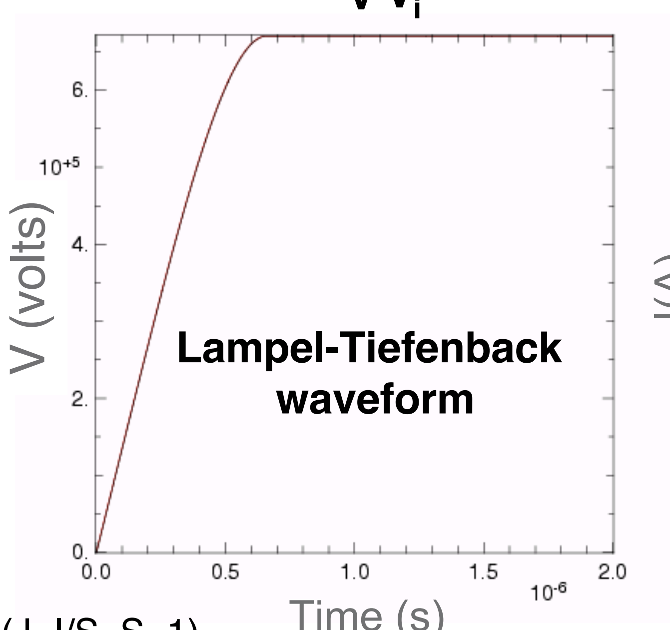


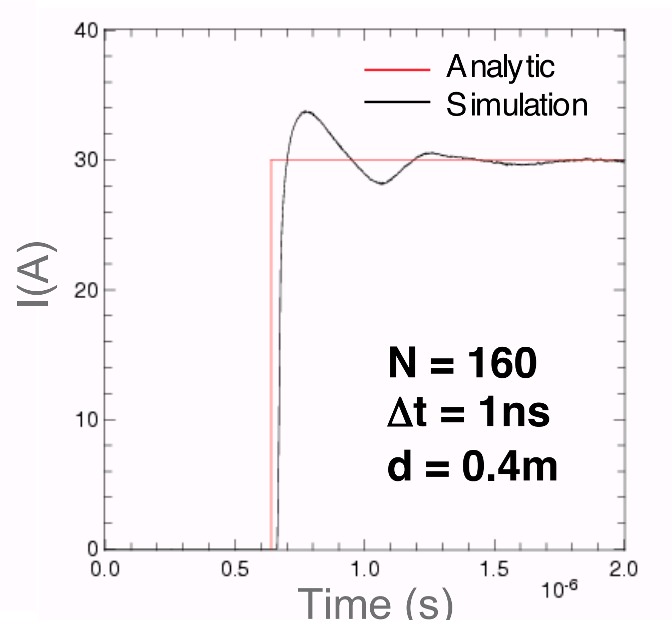
Child-Langmuir solution* + voltage drop between emitter and virtual surface determines current to inject.

$$I = \chi \frac{(V - V_i)^{3/2}}{d_i^2}; \ \chi = \frac{4}{9}\varepsilon_0 \sqrt{\frac{2q}{m}}$$

$$\Rightarrow \Delta Q = Nq = I\Delta t$$

Result

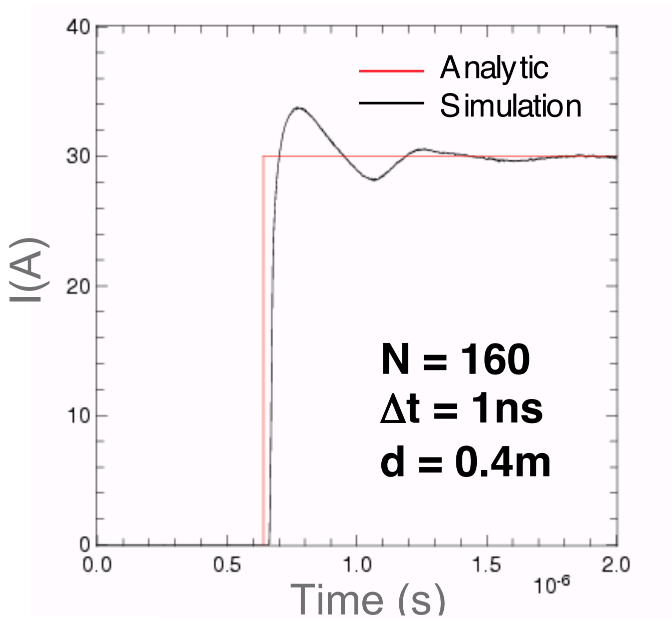


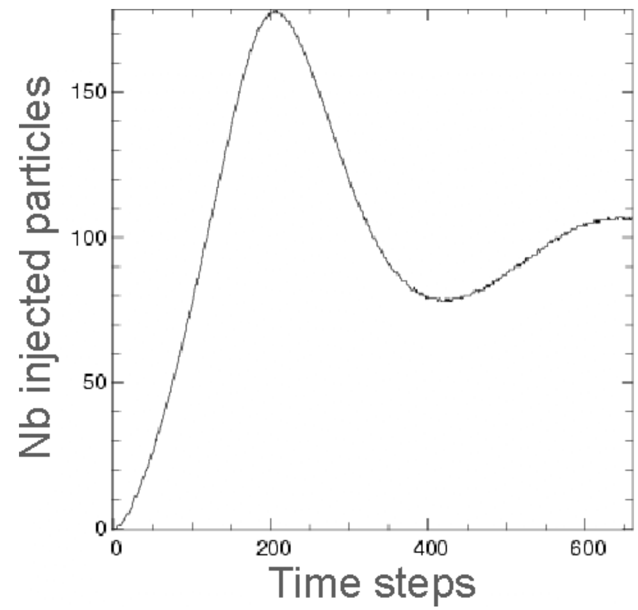


Simulation result exhibits large unphysical oscillation.

*1-D; => J≡I (J=I/S, S=1)

Unphysical oscillation related to Nb particles injected/time step (N_i)

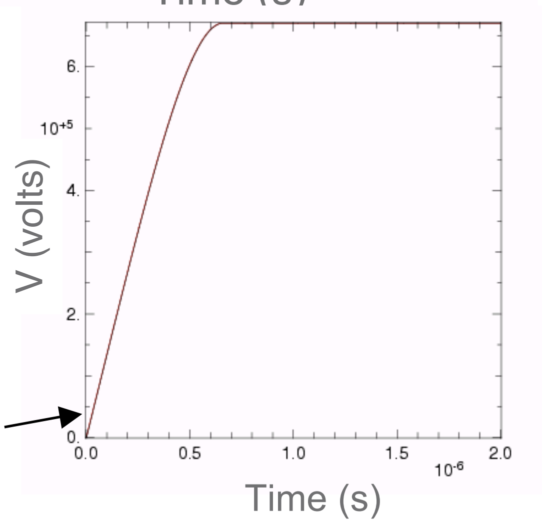




Ideally,

$$\frac{N_i}{\Delta t} = \chi \frac{(V - V_i)^{3/2}}{q d_i^2} = Cste$$

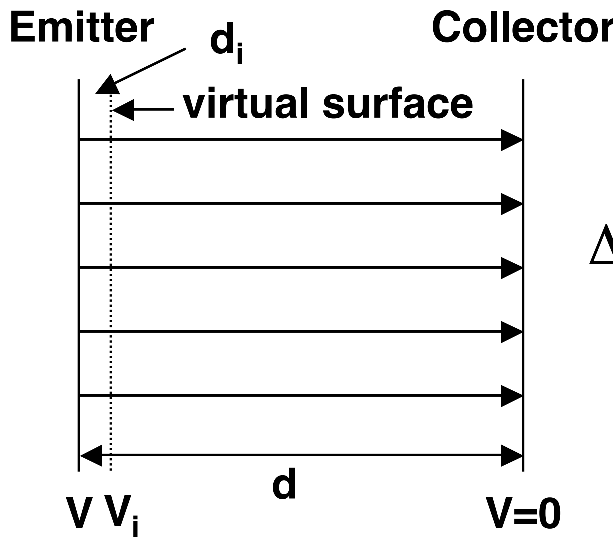
but the driving voltage is a continous function derived analytically.



⇒ Inconsistency due to infinitesimal solution applied in discrete world.

Cure: derive voltage history numerically

Injection algorithm



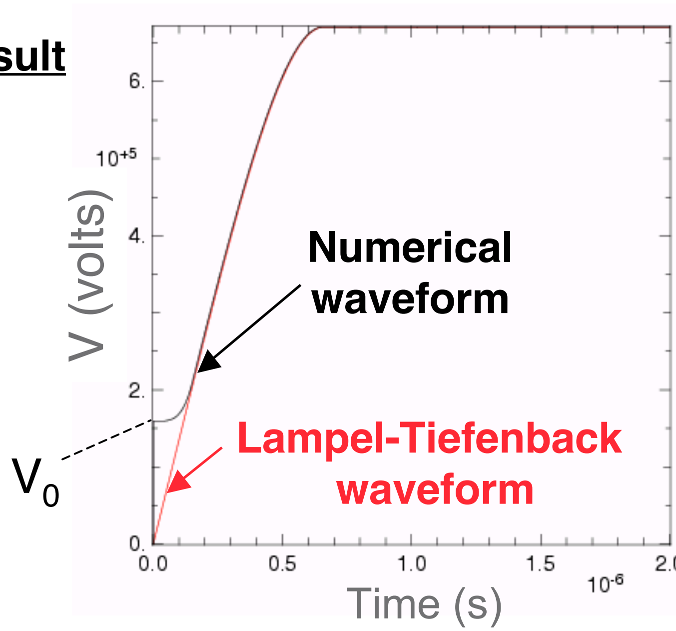
We apply Lampel-Tiefenback method at the discrete level

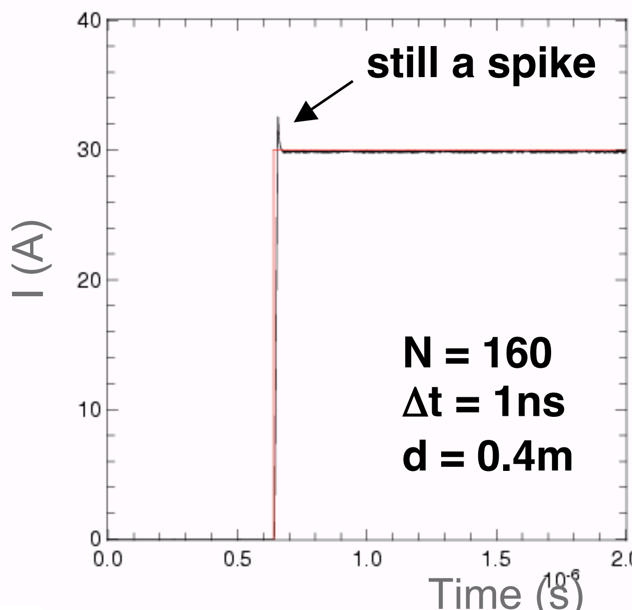
$$\Delta Q = Nq = I\Delta t \Rightarrow V - V_i = \left(\frac{I d_i^2}{\chi}\right)^{2/3}$$

solve for V using linearity of Poisson

$$(V-V_i) = (V-V_i)_{V=0} + (V-V_i)_{\rho=0}$$

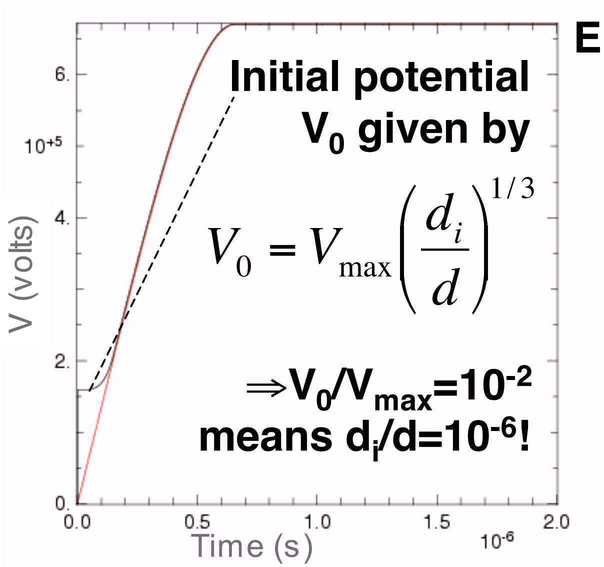
Result

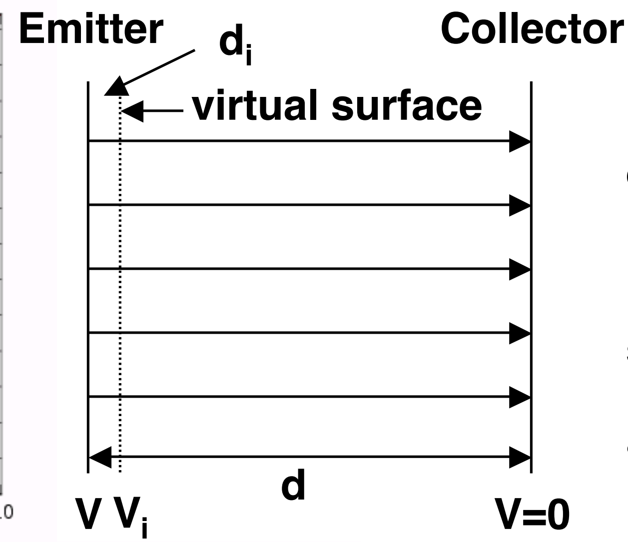




Large unphysical oscillation has been suppressed but there is still a spike. Is it due to initial step V_0 in waveform?

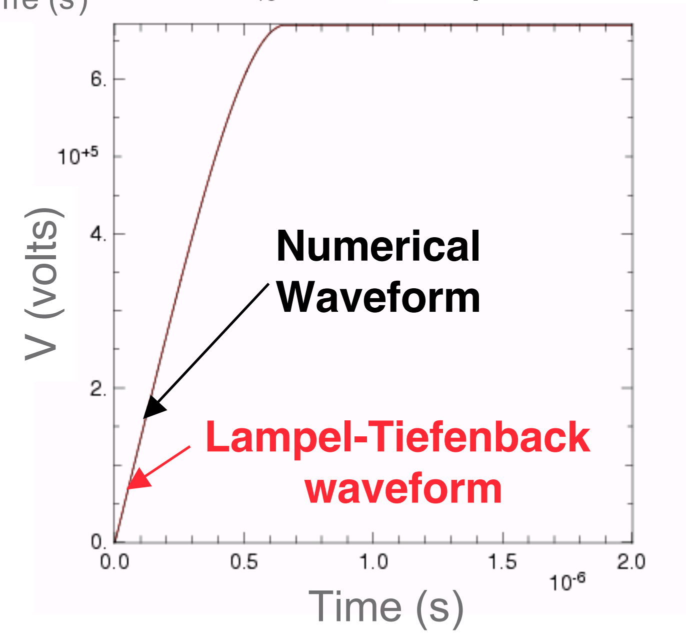
Cure #2: apply irregular gridded patch around emitter.

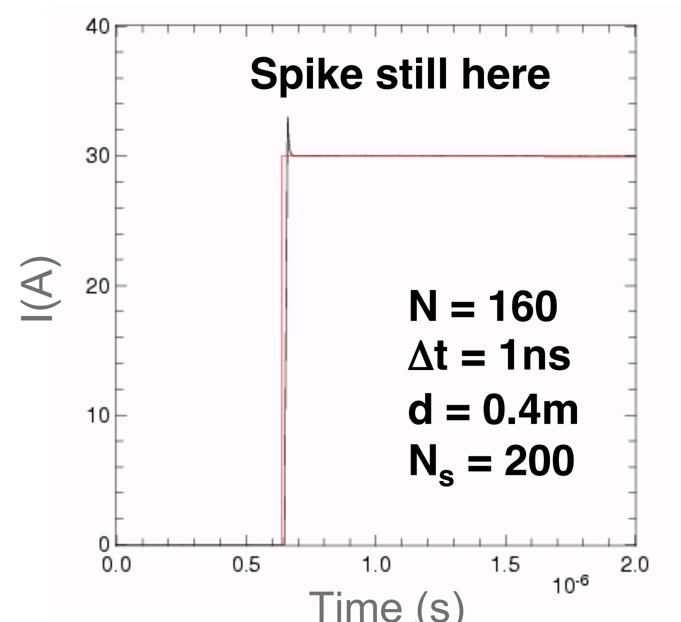




- Apply irregular gridded patch covering d_i
- Mesh sizes such that number of particles per cell is a constant in patch assuming Child-Langmuir solution for $\rho(z)$
- Apply same injection algorithm as before in patch

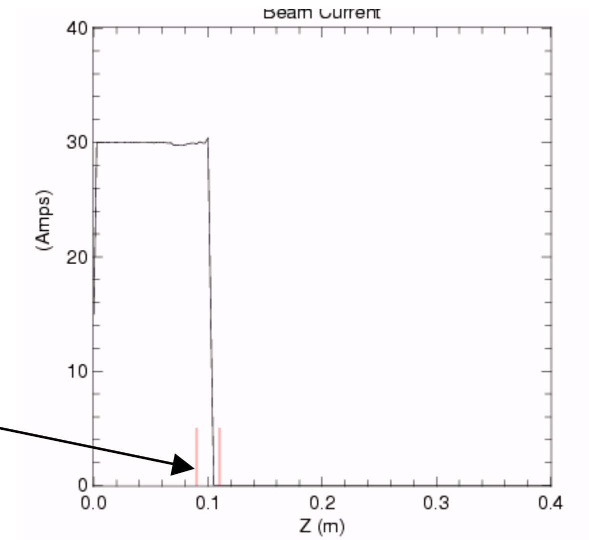
Result



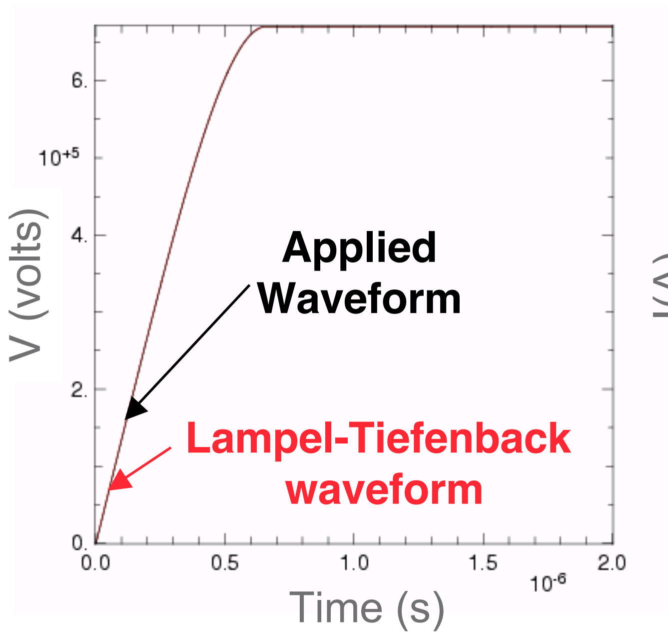


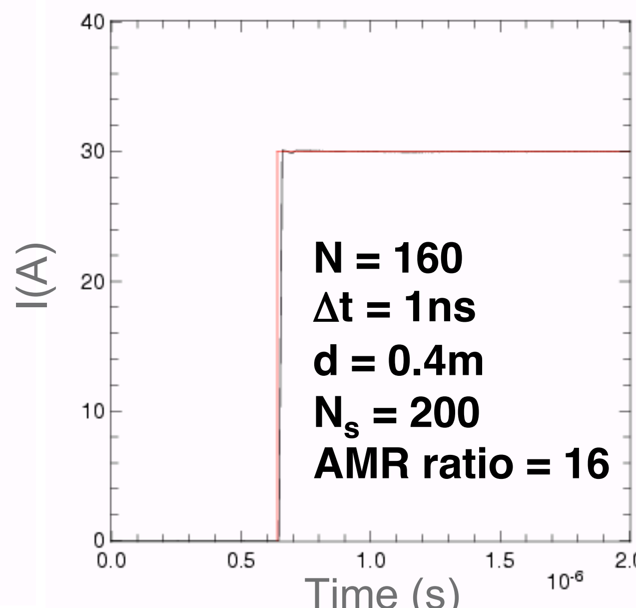
Cure #3: apply regularly gridded patch following front.

An Adaptive-Mesh-Refinement patch Follows the front



<u>Result</u>

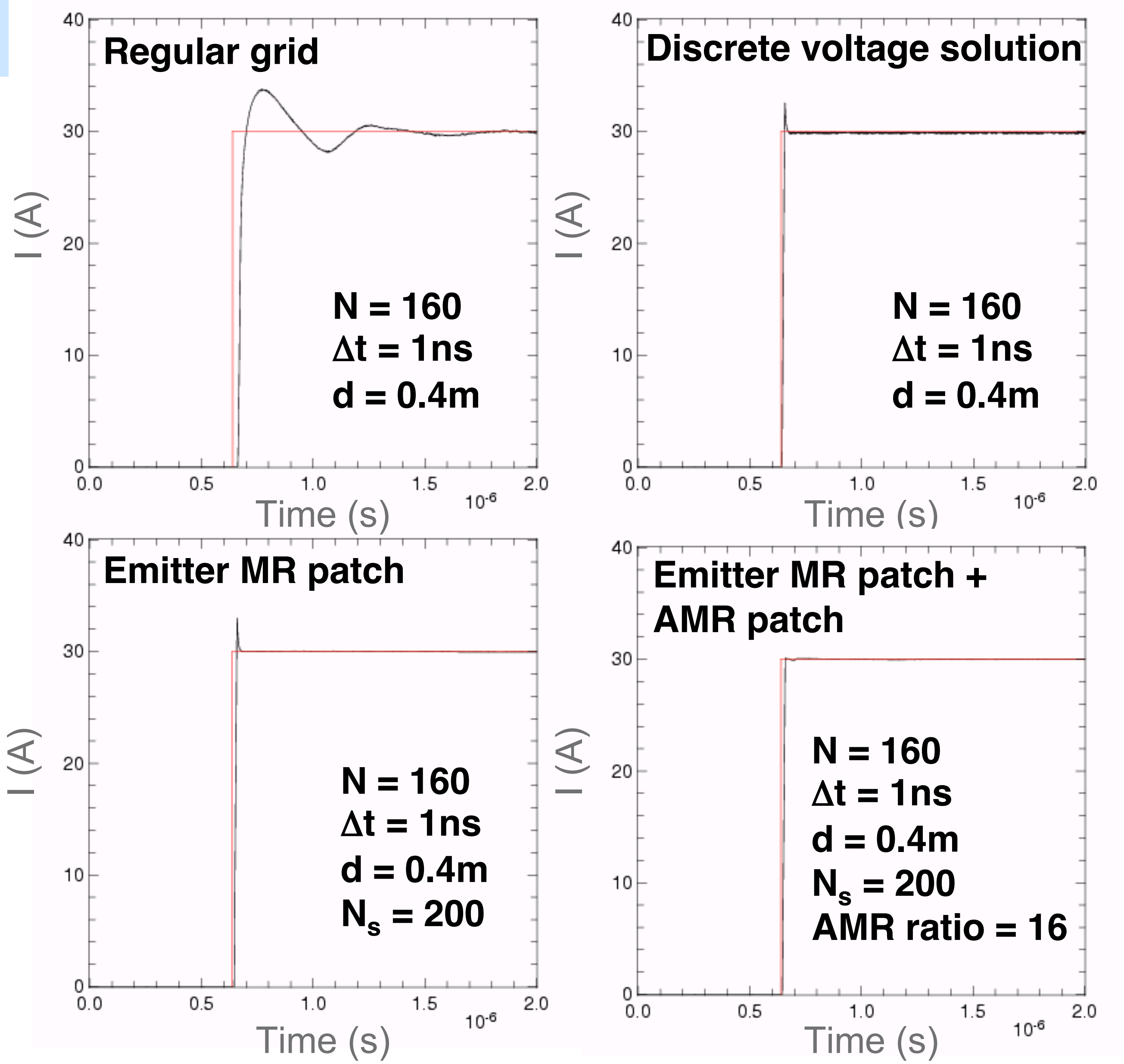




At this point, we declared victory!

Summary

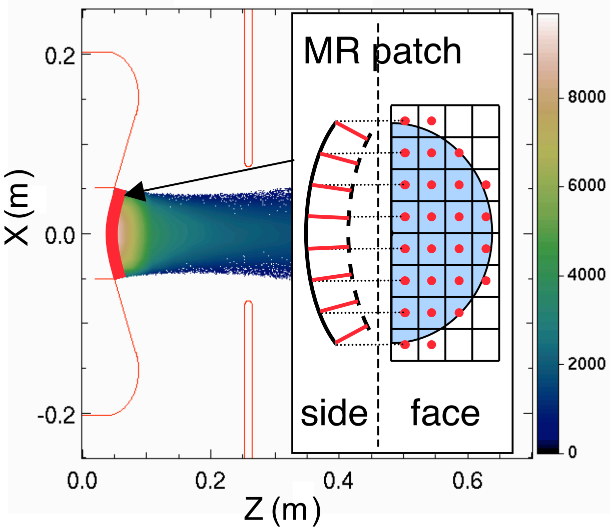
- Discrete voltage solution or MR patch suppressed long wavelength oscillation
- AMR patch suppressed front peak



Extension to three dimensions

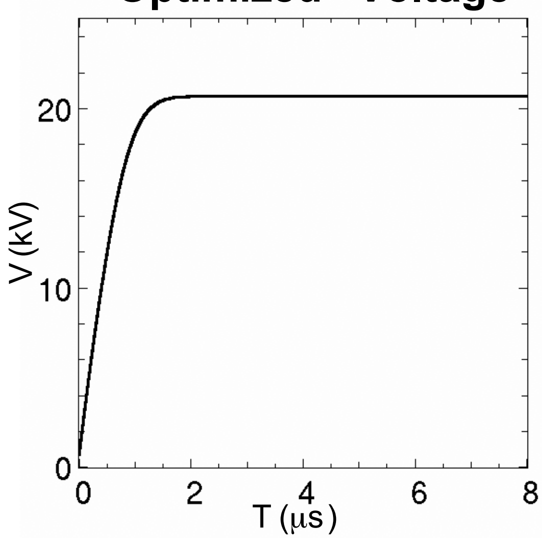
- Specialized 1-D patch implemented in 3-D injection routine, as a 2-D array of 1-D patches.

Ion source diode

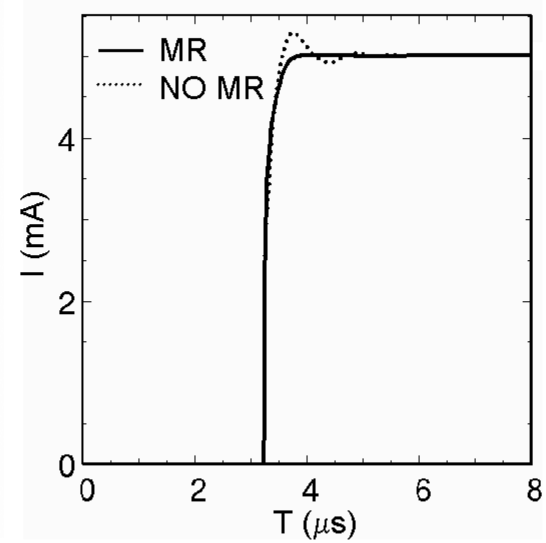


- Extended Lampel-Tiefenback technique to 3-D, and implemented in WARP
  - ➢ predicts a voltage waveform which extracts a nearly flat current at emitter

“Optimized” Voltage

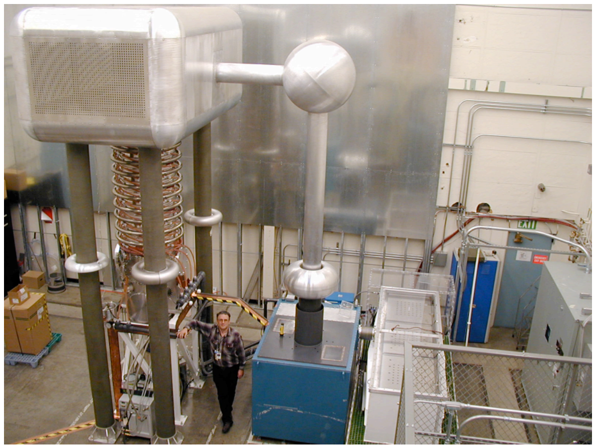


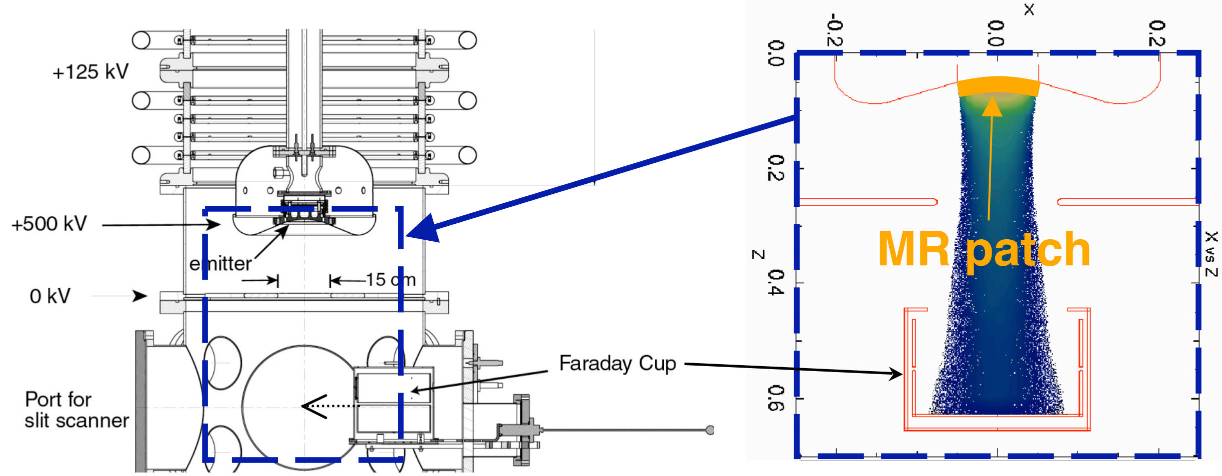
Current at Z=0.62m

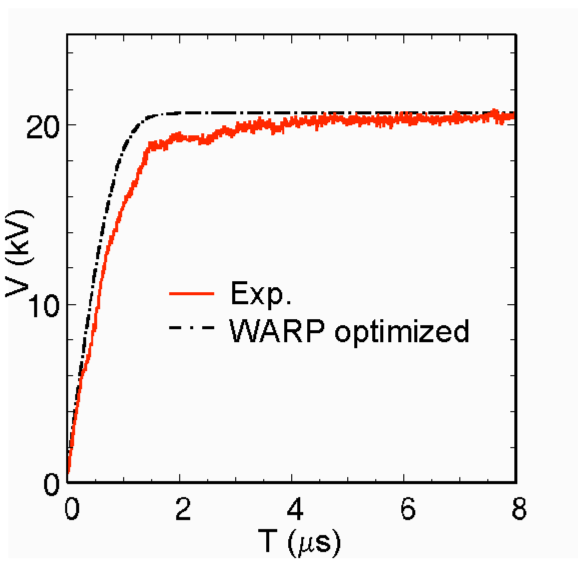


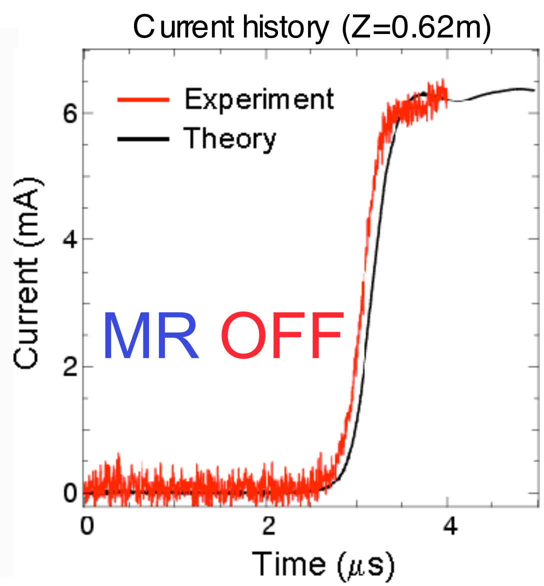
- Without MR, WARP predicts overshoot
- Run with MR predicts very sharp risetime (not square due to erosion)

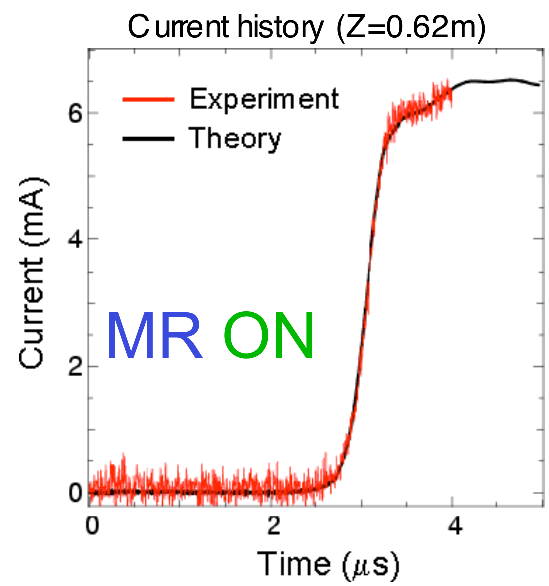
Test of MR patch on modeling of STS500 Experiment.





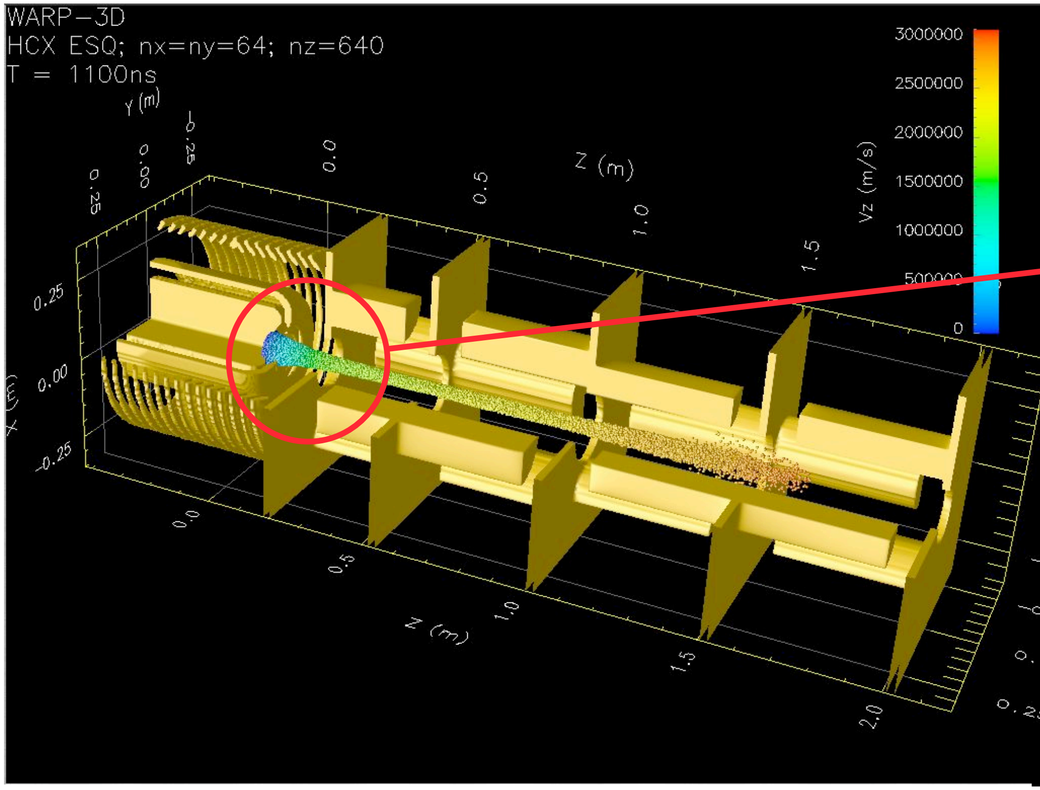


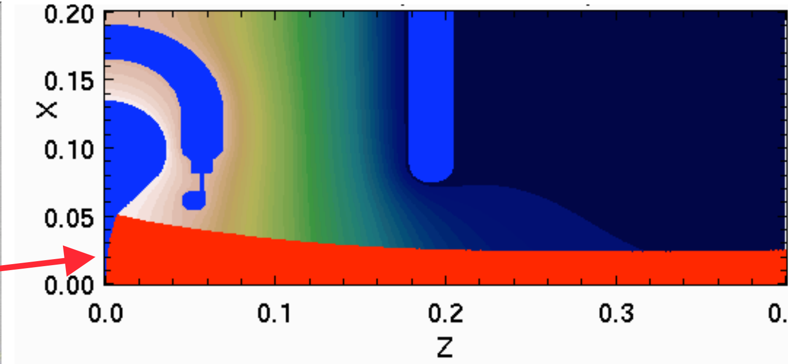




* J.-L. Vay et al, PoP (2003)

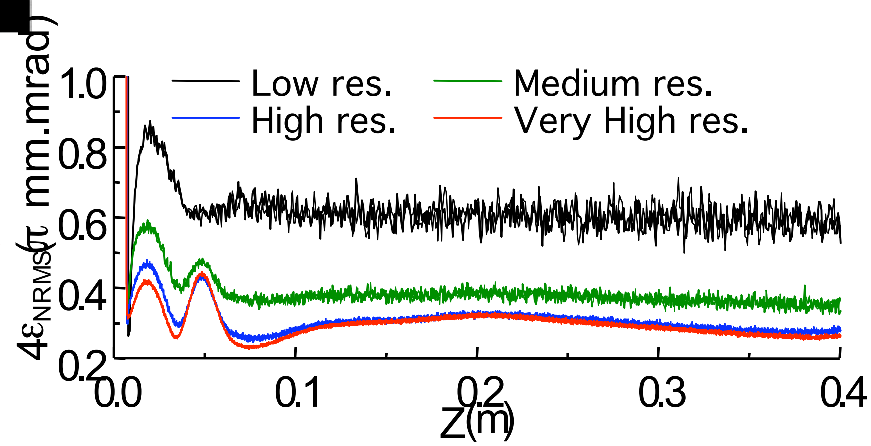
Modeling of source critical - determines initial shape of beam.



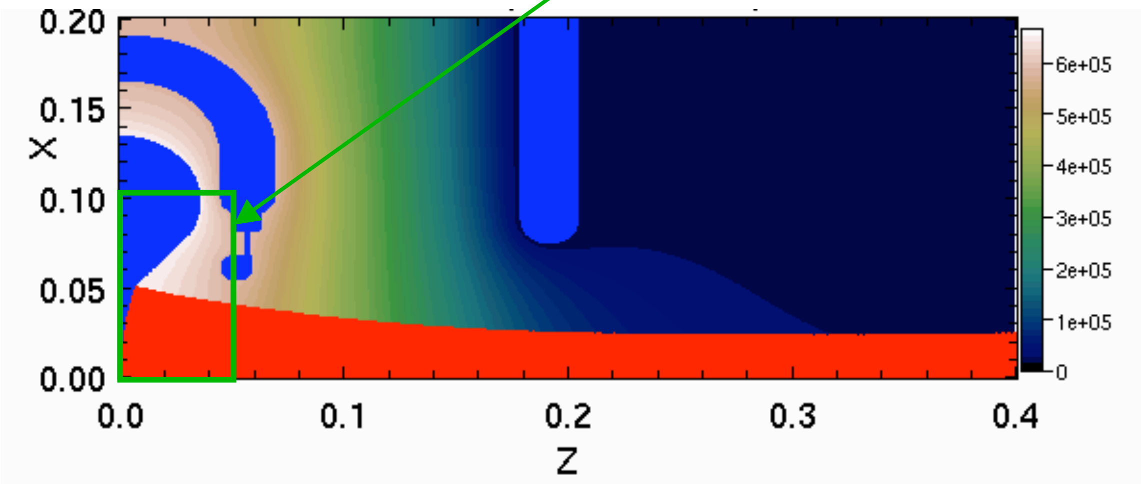


Run	Grid size	Nb particles
Low res.	56x640	~1M
Medium res.	112x1280	~4M
High res.	224x2560	~16M
Very High res.	448x5120	~64M

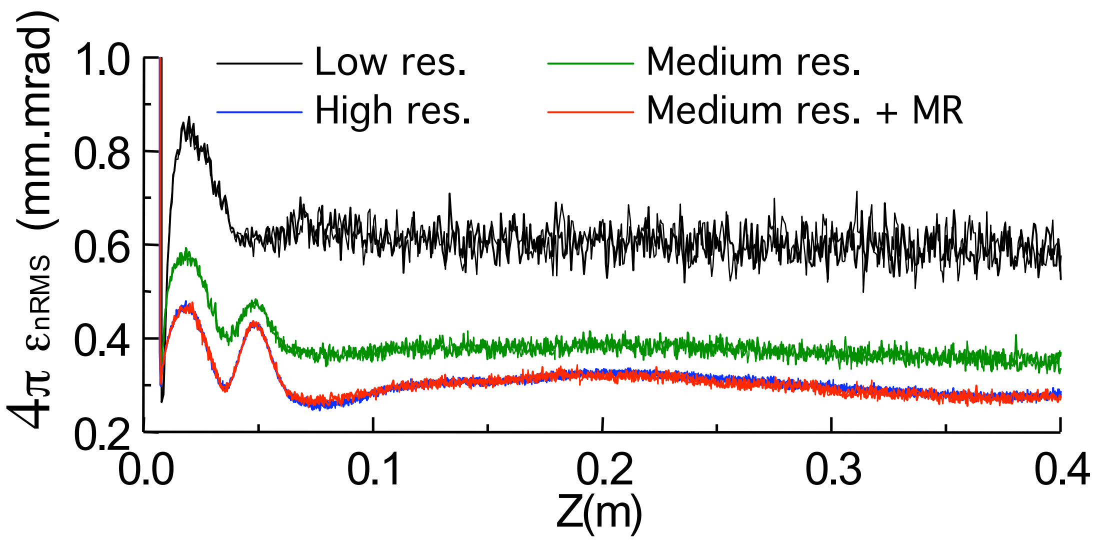
WARP-RZ (axi-symmetric) simulations show that a fairly high resolution is needed to reach convergence



First MR attempt - 1 MR block surrounding emitter.



Refining around the emitter area is enough to recover emittance from converged high-resolution case.

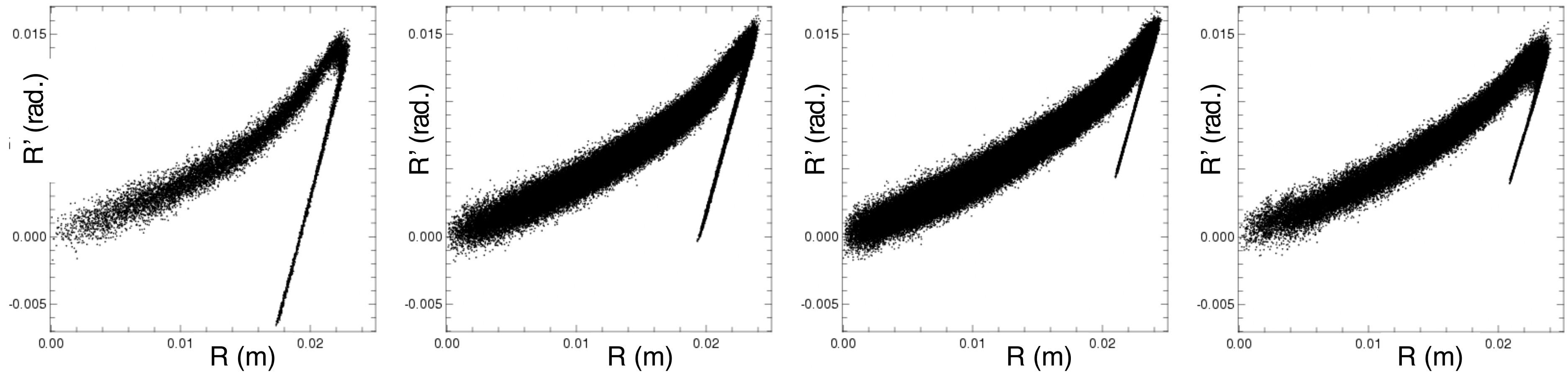


Run	Grid size	Nb particles
Low res.	56x640	~1M
Medium res.	112x1280	~4M
High res.	224x2560	~16M
Medium res. + MR	112x1280	~4M

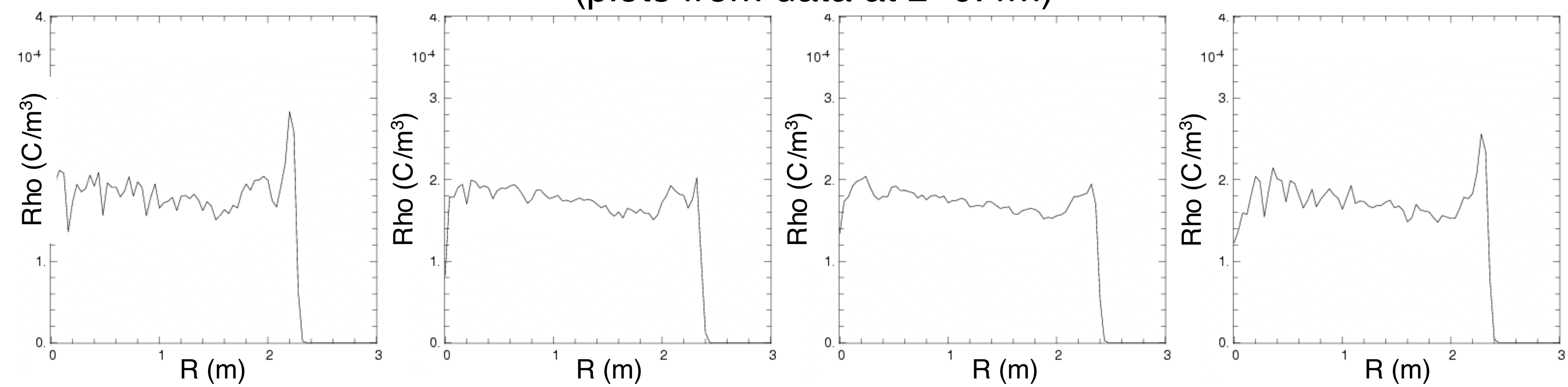
First MR attempt - 1 MR block surrounding emitter (2).

However, it is not enough for recovering details of distribution.

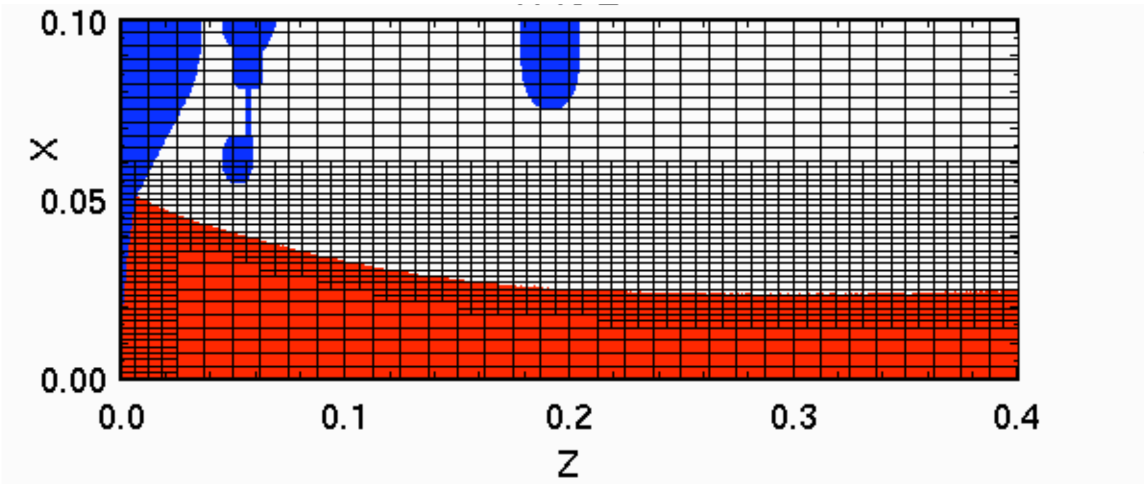
Low res. | Medium res. | High res. | Medium res. + MR



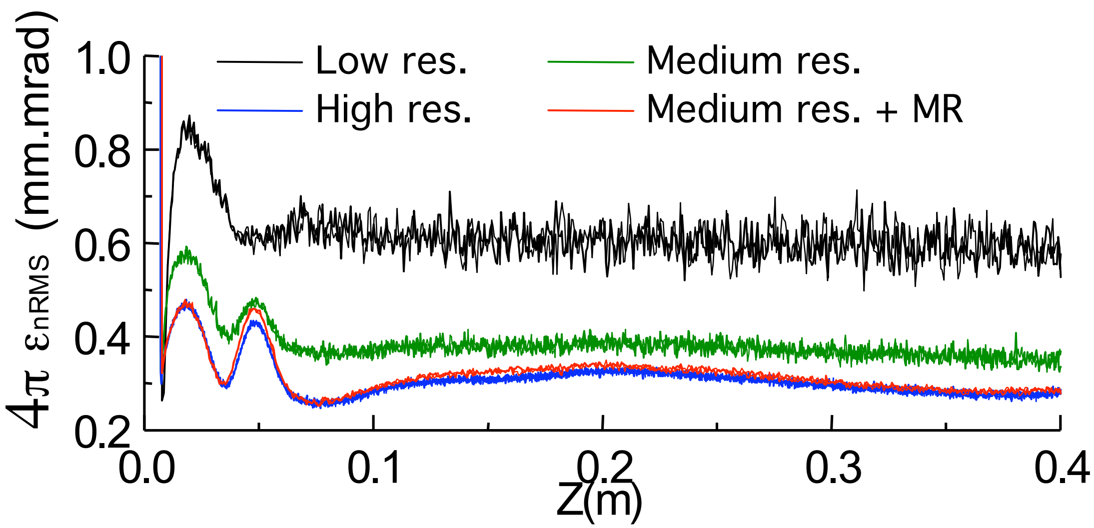
(plots from data at z=0.4m)



Second attempt - 1 MR block with adaptive excavation.



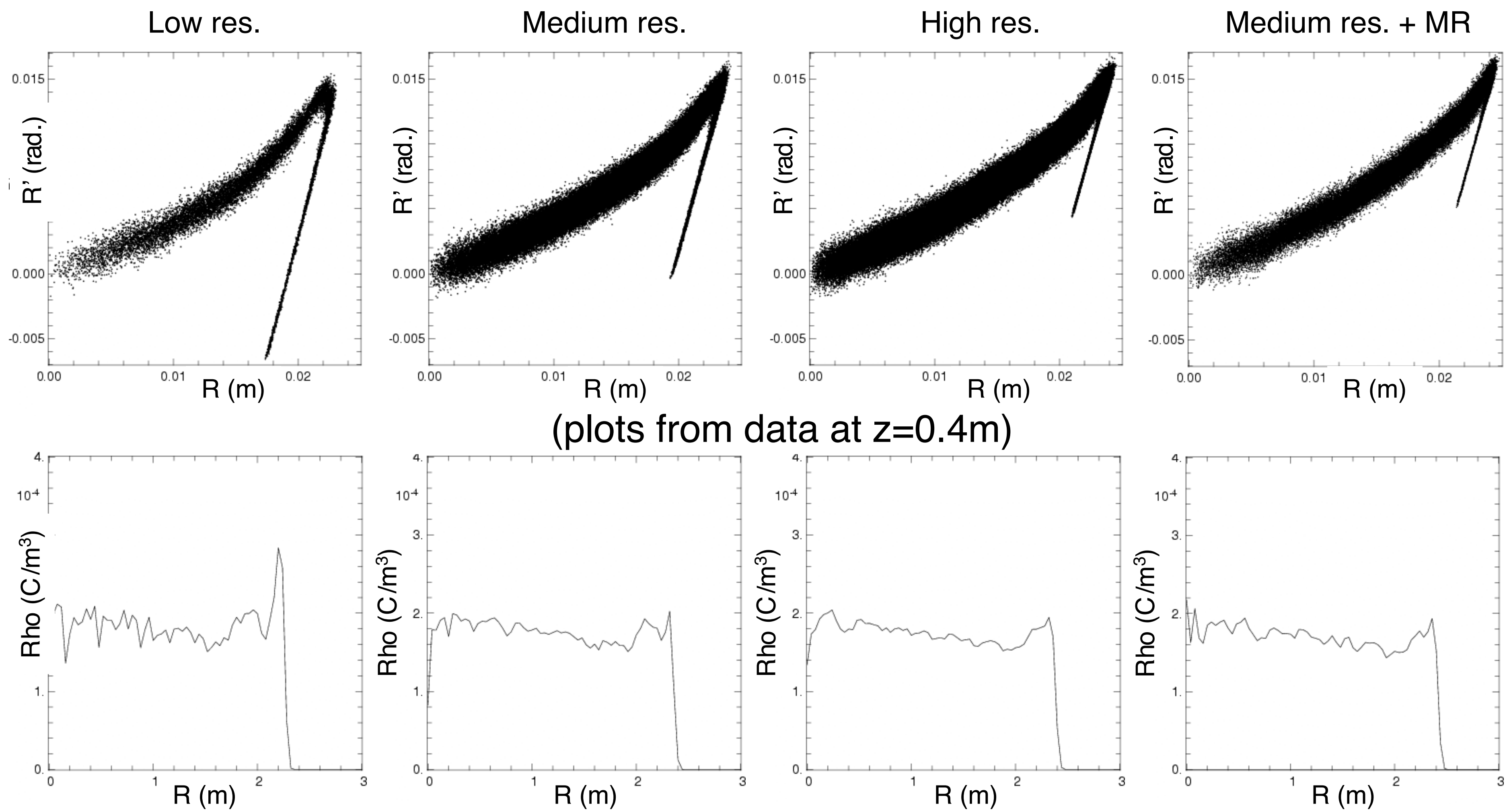
Emittance recovered, again.



Run	Grid size	Nb particles
Low res.	56x640	~1M
Medium res.	112x1280	~4M
High res.	224x2560	~16M
Medium res. + MR	112x1280	~4M

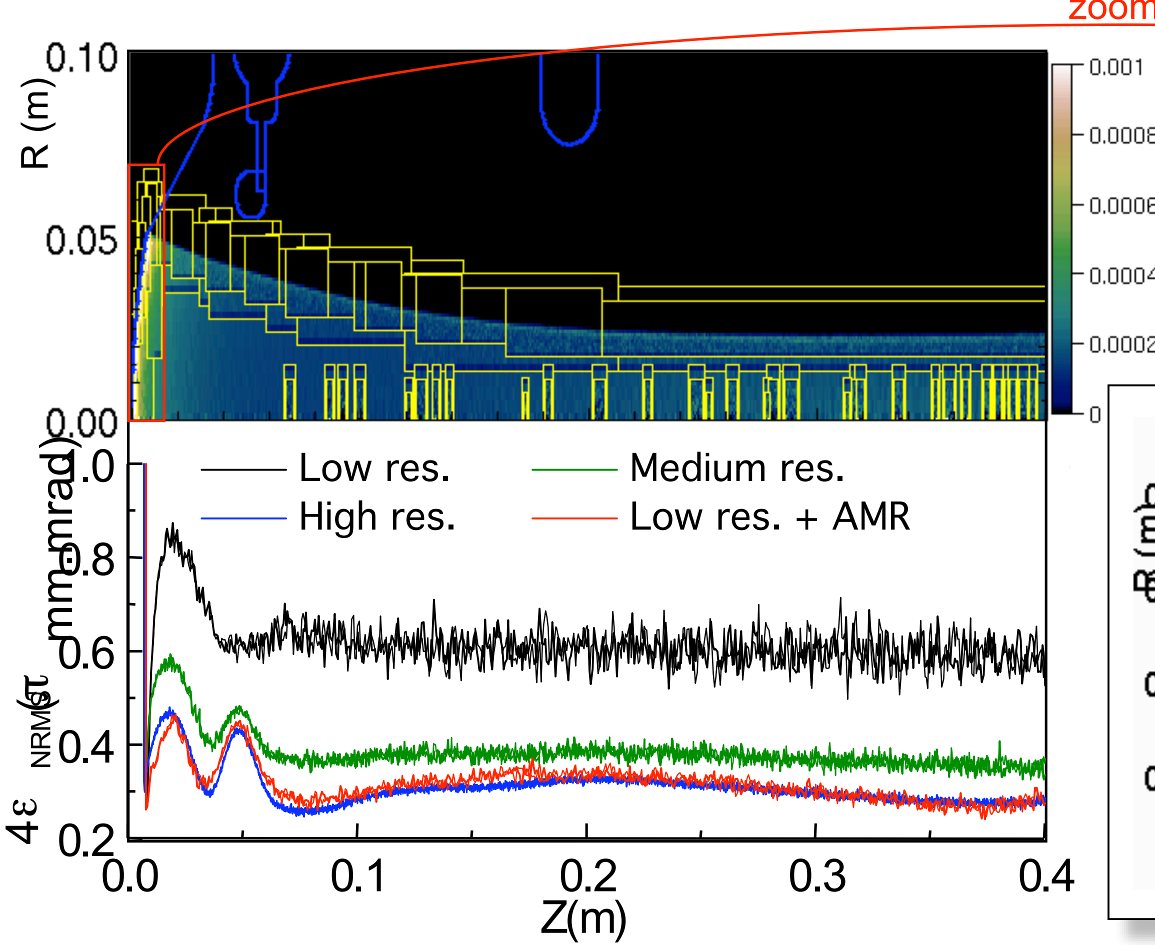
Second attempt - 1 MR block with adaptive excavation (2).

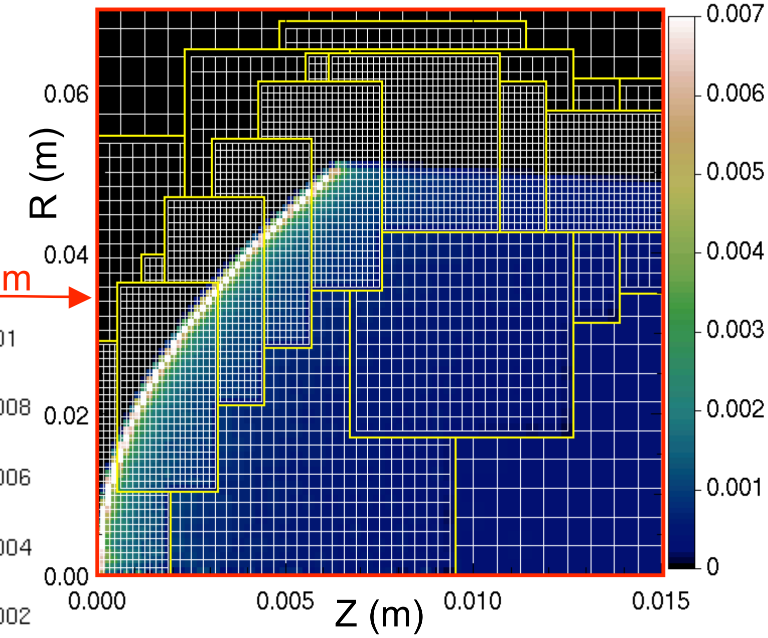
Refining emission are AND beam edge sufficient for recovering details of distribution.

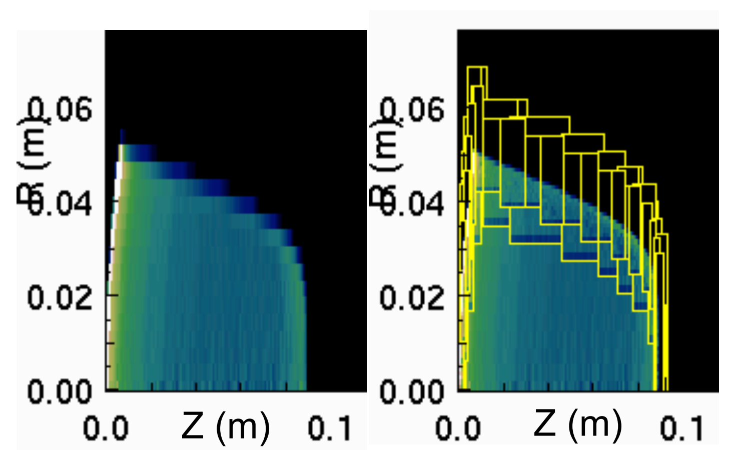


Full AMR implementation: speedup ~10.5

Run	Grid size	Nb particles
Low res.	56x640	~1M
Medium res.	112x1280	~4M
High res.	224x2560	~16M
Low res. + AMR	56x640	~1M







Refinement of gradients: emitting area, beam edge and front.

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Study of e-cloud in LHC FODO cell

The problem:

Simulate "multibunch, multiturn" passage of beam through FODO cell (~100 m):

- dipoles
- quadrupoles
- drifts

Electrons $\Leftarrow$ synchrotron radiation, secondary emission

Study:

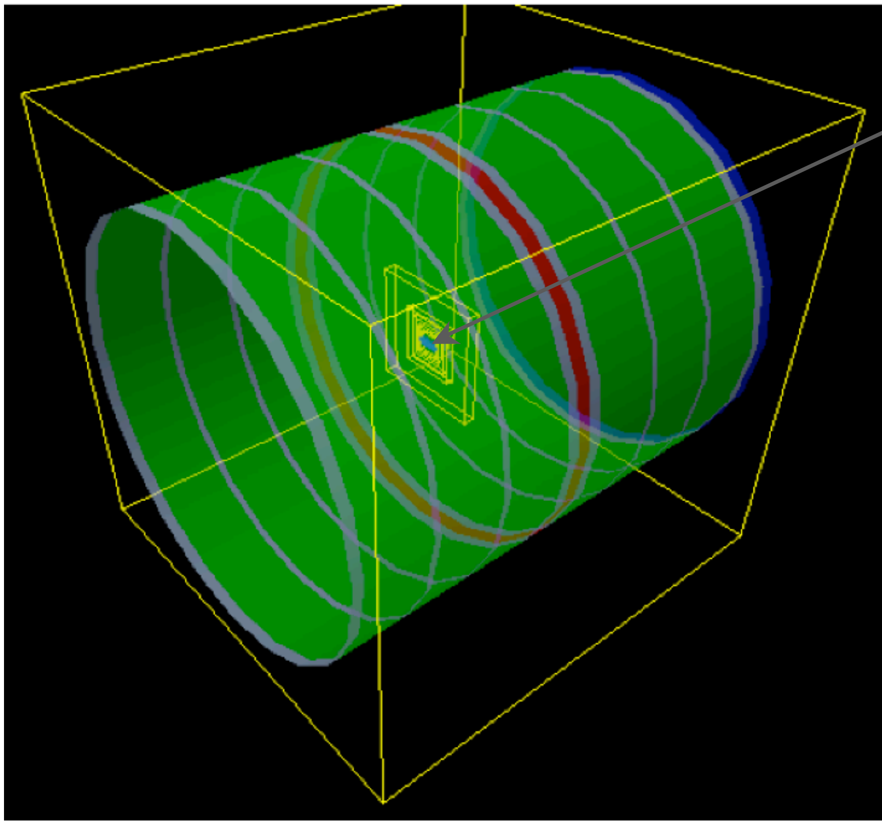
Electron accumulation and trapping in quads

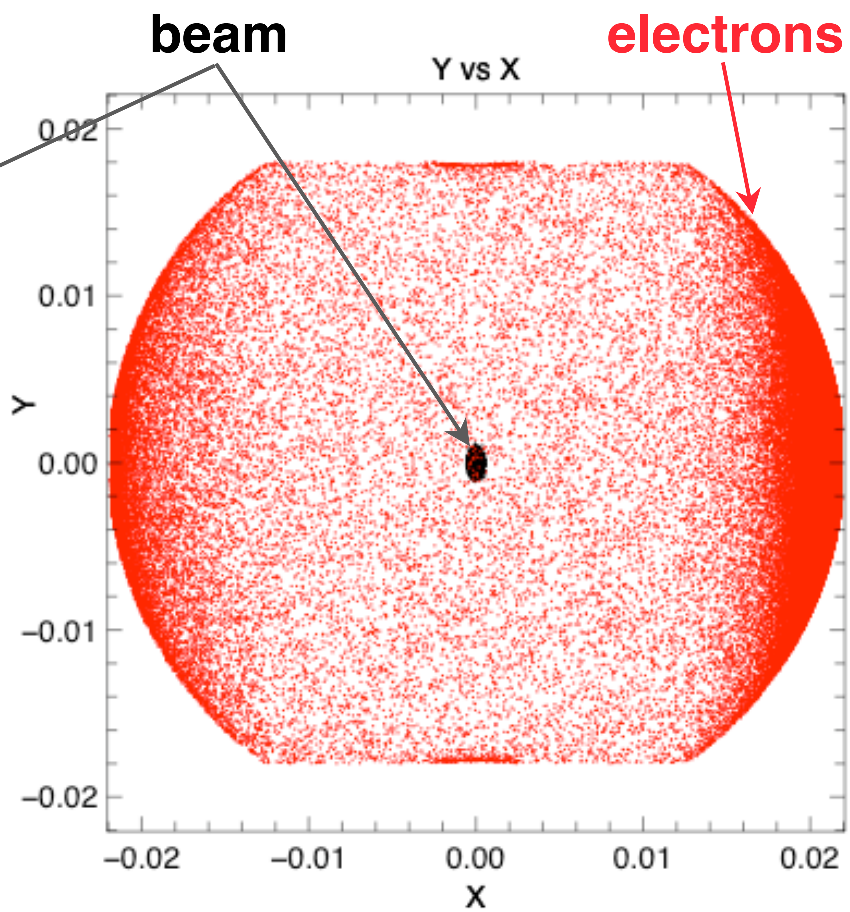
Power deposition from electrons

First try with one bunch in periodic FODO cell.

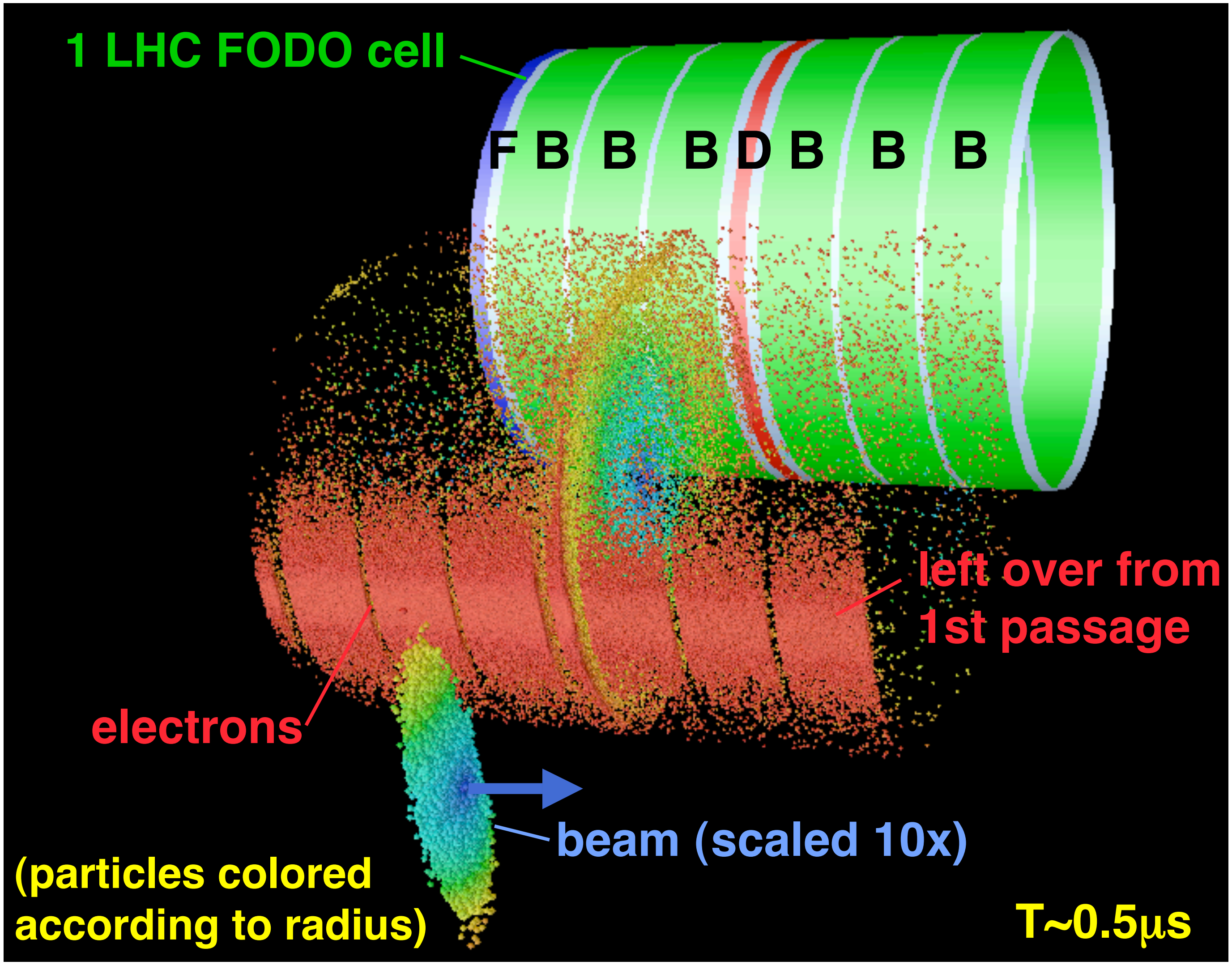
Frame 2nd passage of bunch through cell - 2

- We use actual LHC pipe shape: beam size << pipe radius
- Mesh Refinement provides speedup of **x20,000** on field solve





Frame 2nd passage of bunch through cell - 1



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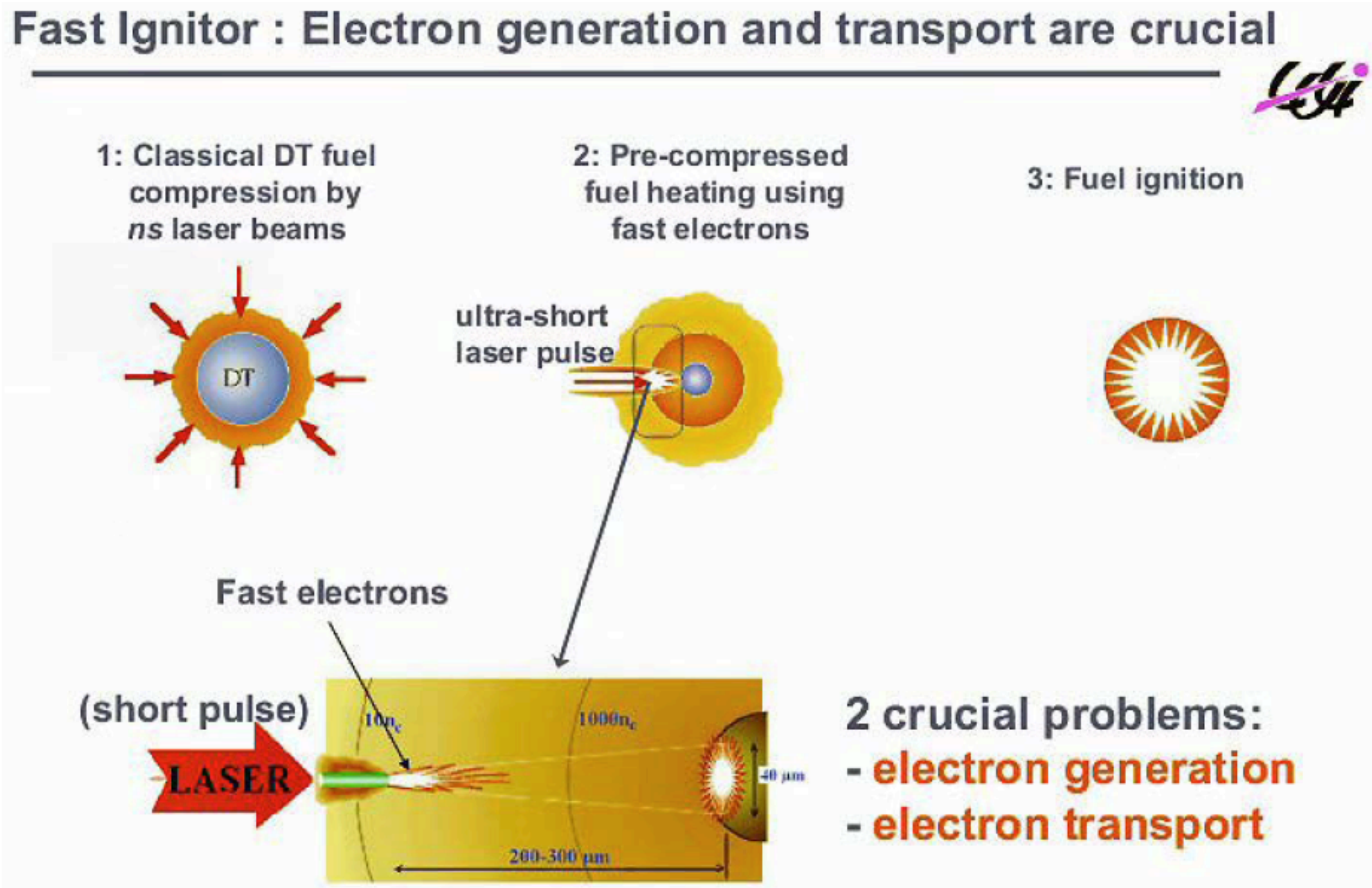
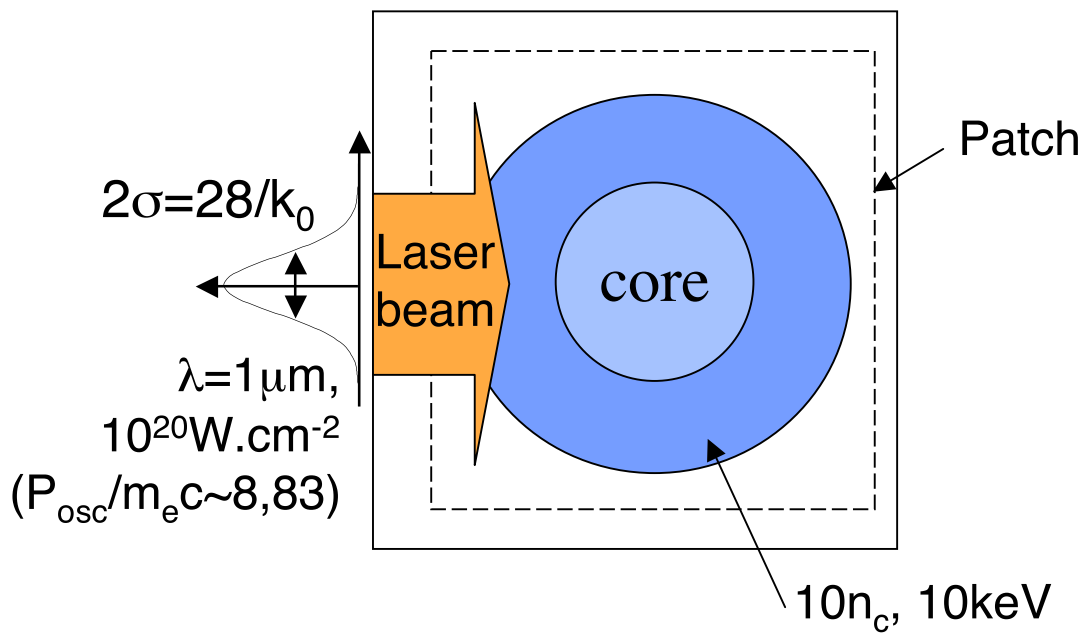
A cartoon of fast ignition.



Laser-plasma interaction in the context of fast ignition

- **A laser impinges on a cylindrical target which density is far greater than the critical density.**
- **The center of the plasma is artificially cooled to simulate a cold high-density core.**
- **Patch boundary surrounds plasma. Laser launched outside the patch.**



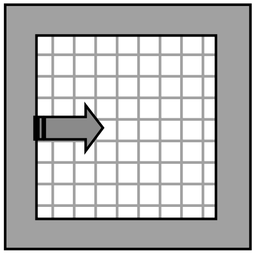
- **Implemented new MR technique in EM PIC code Emi2d (E. Polytech.)**

EMI2D code

- **PIC electromagnetic 2D, cubic splines (- noise, + stable), Esirkepov exact current deposition scheme**
- **Boundary conditions: open system**
  - **particles**

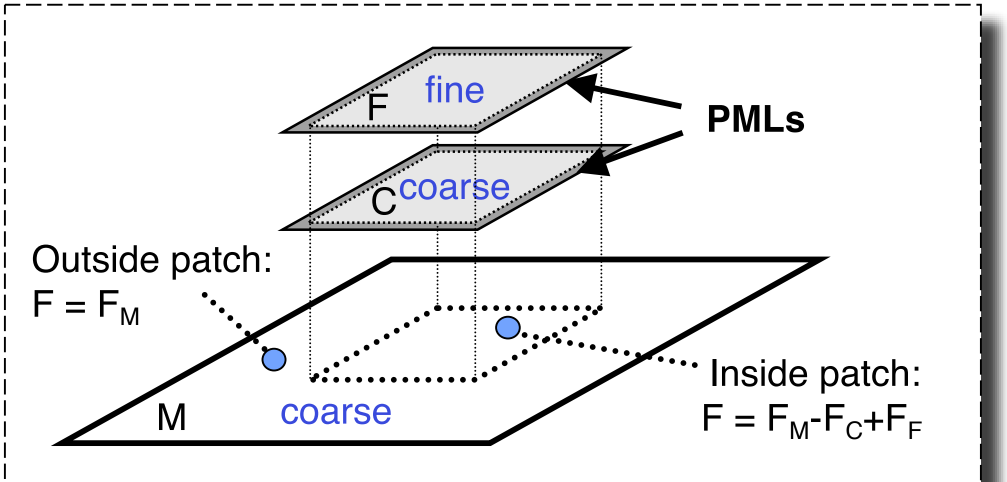
    ions leave the box freely

    electrons reflected until an ion exit (overall charge conserved)
  - **EM fields: absorbing layer ("Asymmetric PML"*) + incoming wave**



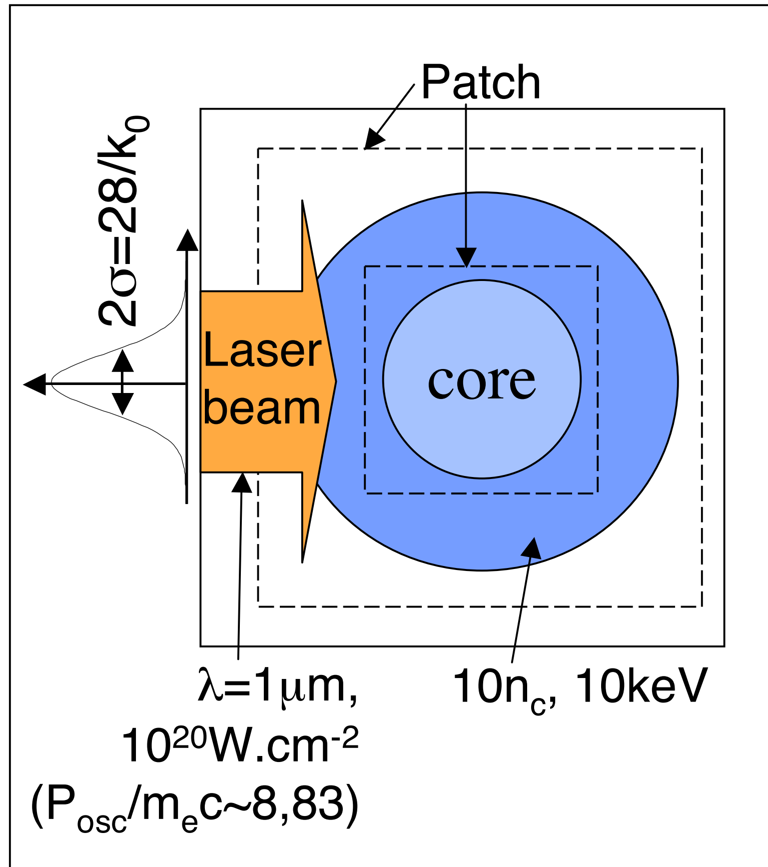
*** Vay, *JCP* (2002)**

New MR method implemented in EM PIC code Emi2d



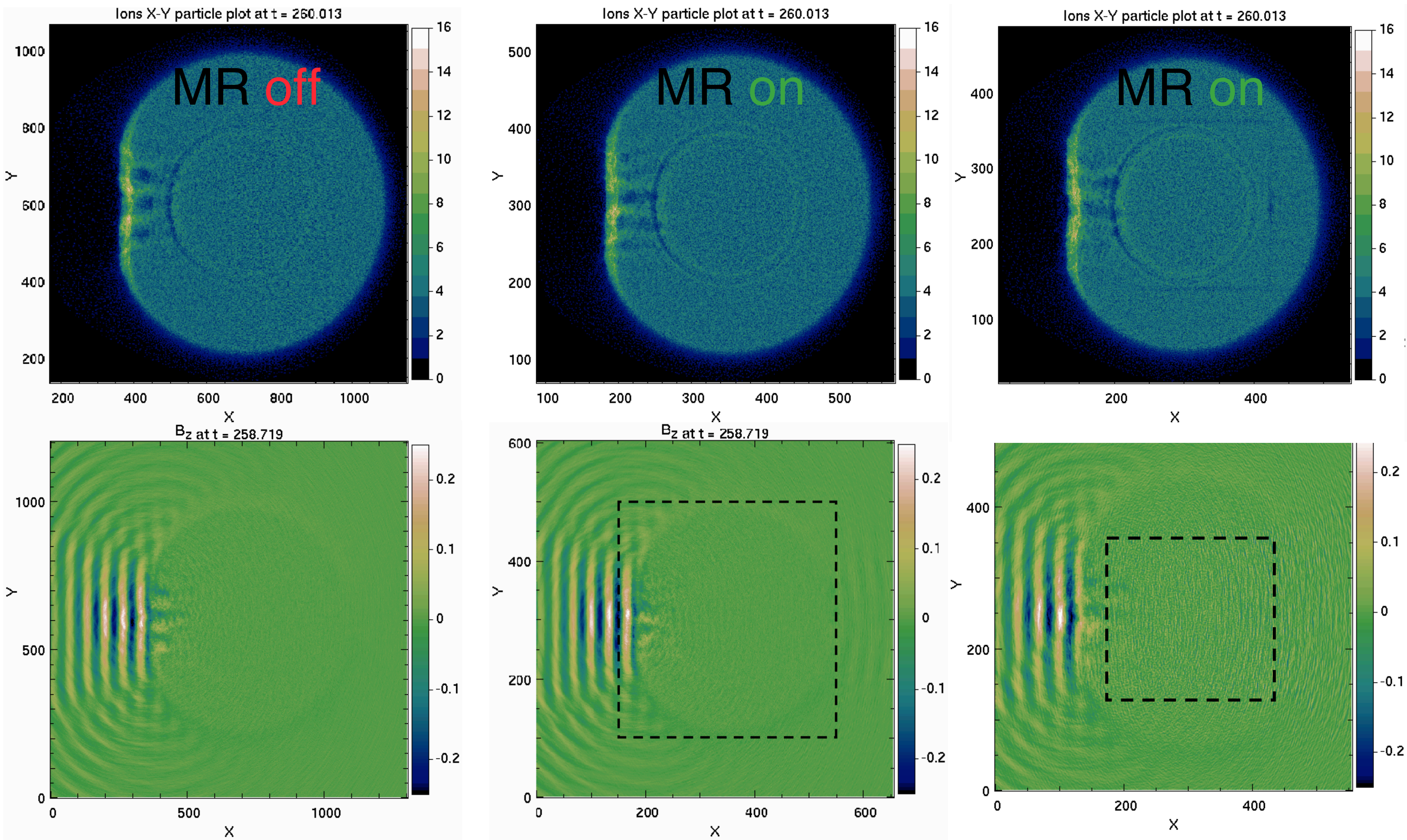
Mesh refinement by substitution*

Applied to Laser-plasma interaction in the context of fast ignition



* J.-L. Vay, J.-C. Adam, A. Heron, CPC (2004)

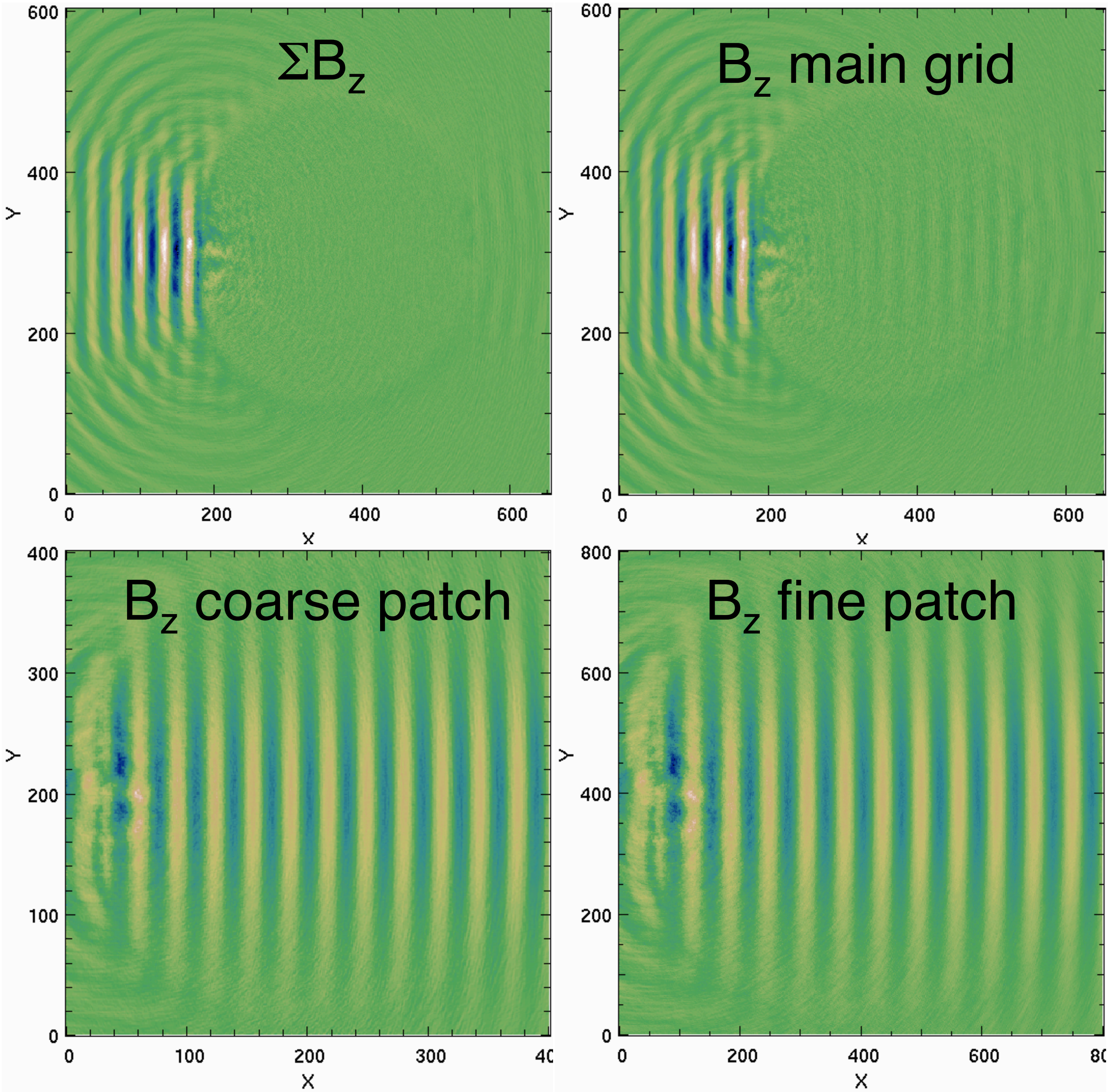
Comparison patch on/off

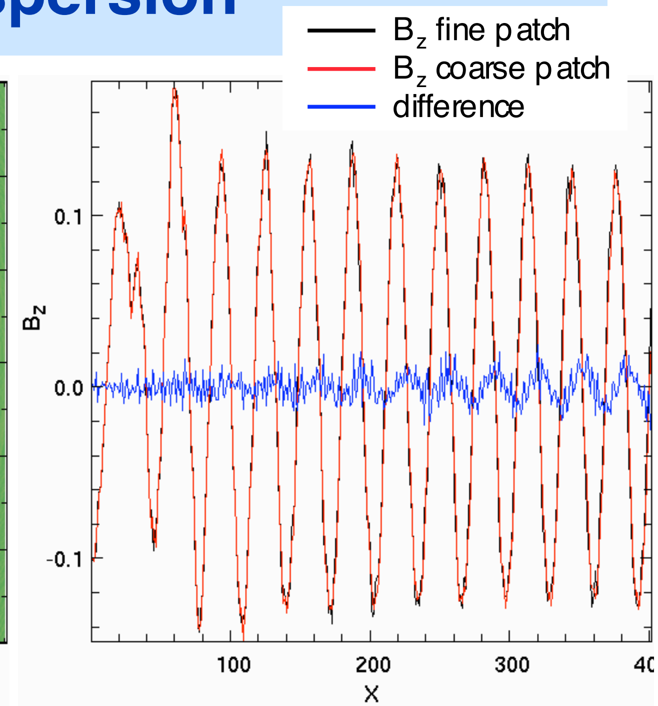


same results except for:

- small residual incident laser at exit of patch when patch englobes target
- dip in density on patch border when patch inside target

Partial cancellation due to numerical dispersion

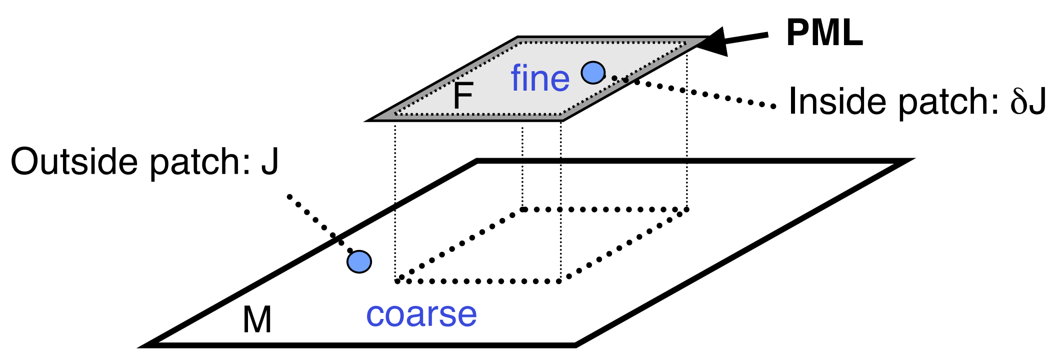




- main grid: laser + plasma response + residual
- patches: plasma response at two slightly different velocities

Possible paths for better scheme

- **Use less dispersive Maxwell solver**
- **Inject residual of waves on main grid at patch interface**
- **Do not use coarse patch and solve on fine patch with source term δJ as a correction to J**



- **Go back to usual scheme with a hole in the main grid**
  - **put PML inside hole and on fine patch border**
  - **couple using clean cross-injections**

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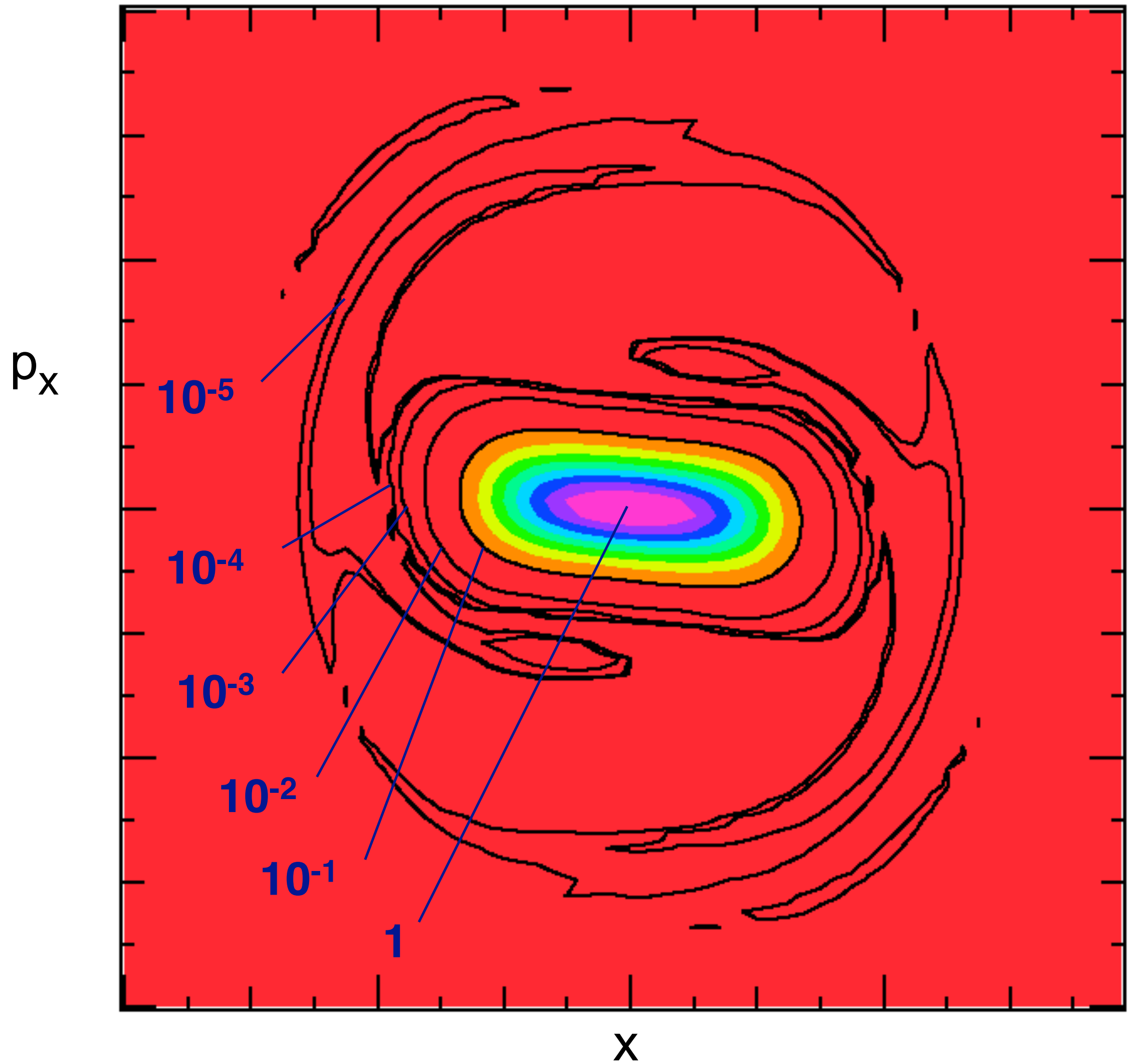
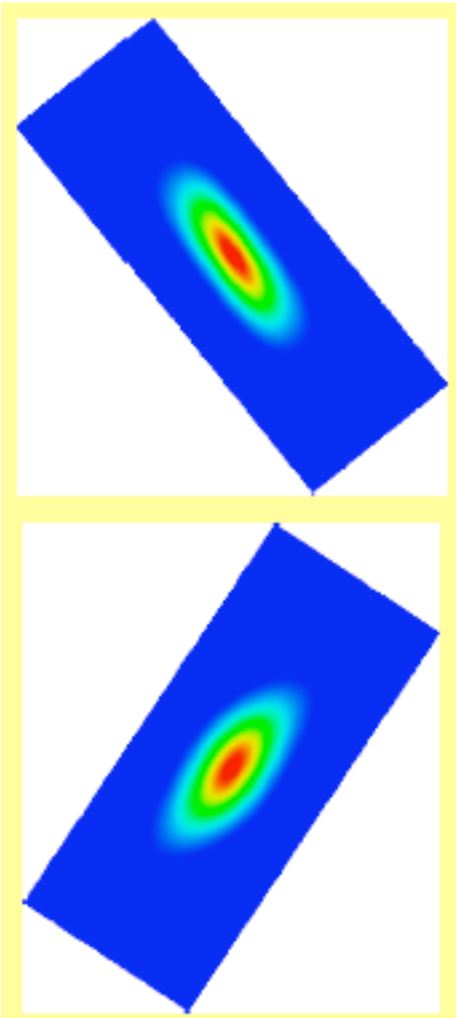
Solution of Vlasov equation on a grid in phase space offers low noise, large dynamic range for beam halo studies



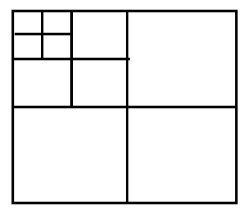
4D Vlasov testbed (with constant focusing) showed structure of the halo in a density-mismatched beam

New ideas: moving grid to model time-dependent applied field, AMR-Vlasov to resolve fine structures



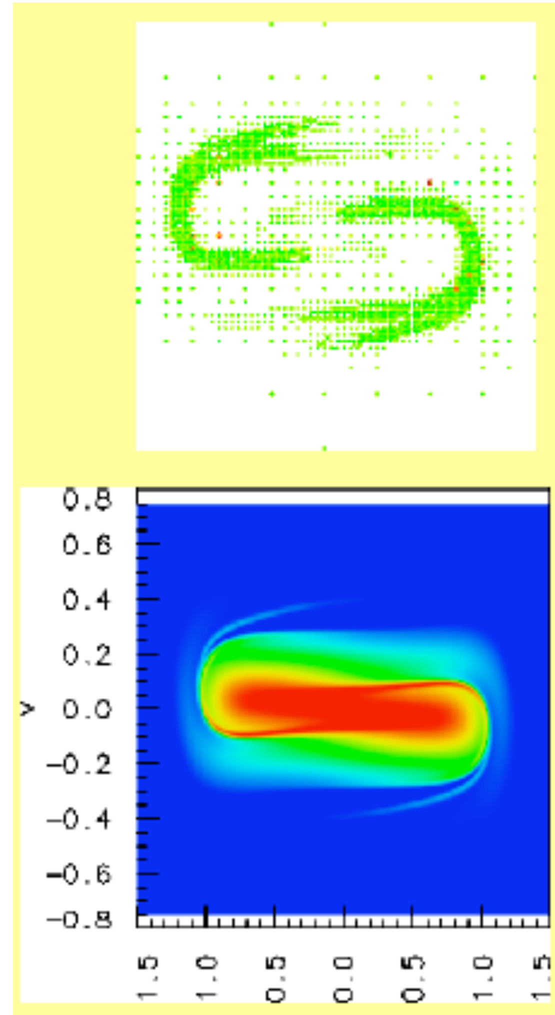
moving phase-space grid,
based on non-split
semi-Lagrangian advance
[E. Sonnendrucker,
F. Filbet, A. Friedman,
E. Oudet, J.-L. Vay, *CPC*,
2004]

⇐



⇒

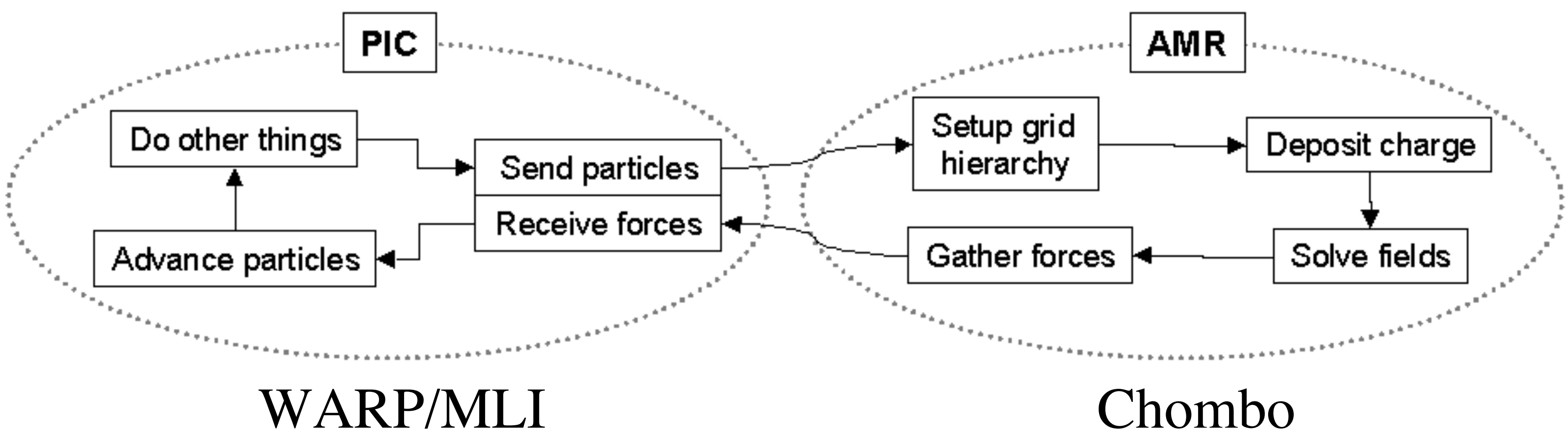
adaptive mesh [M. Gutnic, M. Haefele, I. Paun , E Sonnendrucker, CPC 2004]



3.3 - Development of AMR library for PIC at LBNL

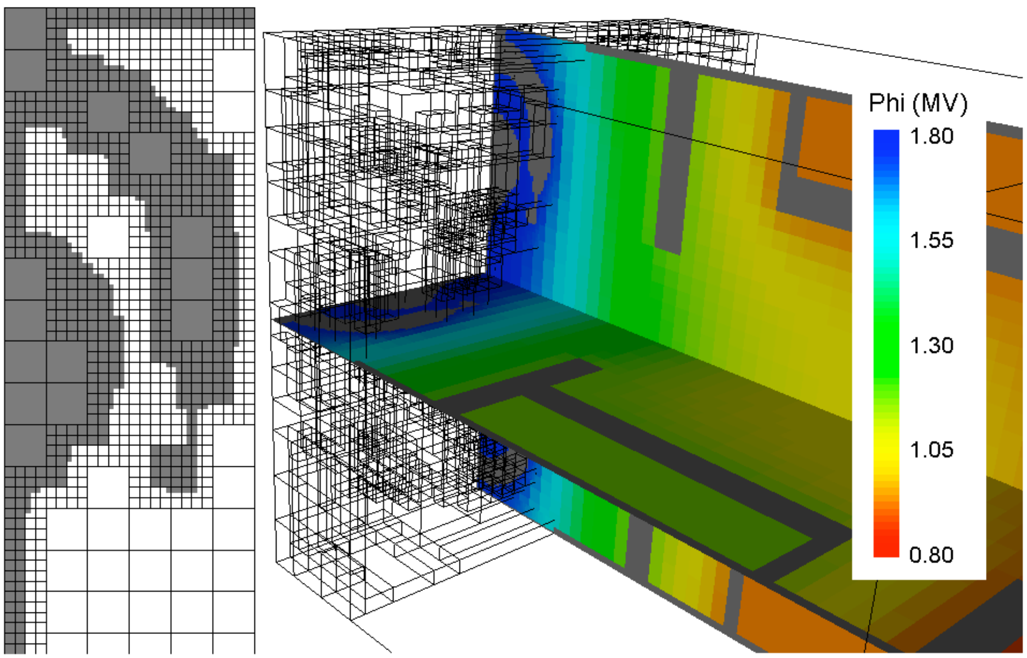
Effort to develop AMR library for PIC at LBNL

- **Researchers from AFRD (PIC) and ANAG (AMR-Phil Colella's group) collaborate to provide a library of tools that will give AMR capability to existing PIC codes (on serial and parallel computers)**
- **The base is the existing ANAG's AMR library Chombo (http://seesar.lbl.gov/anag/chombo)**
- **The way it works**

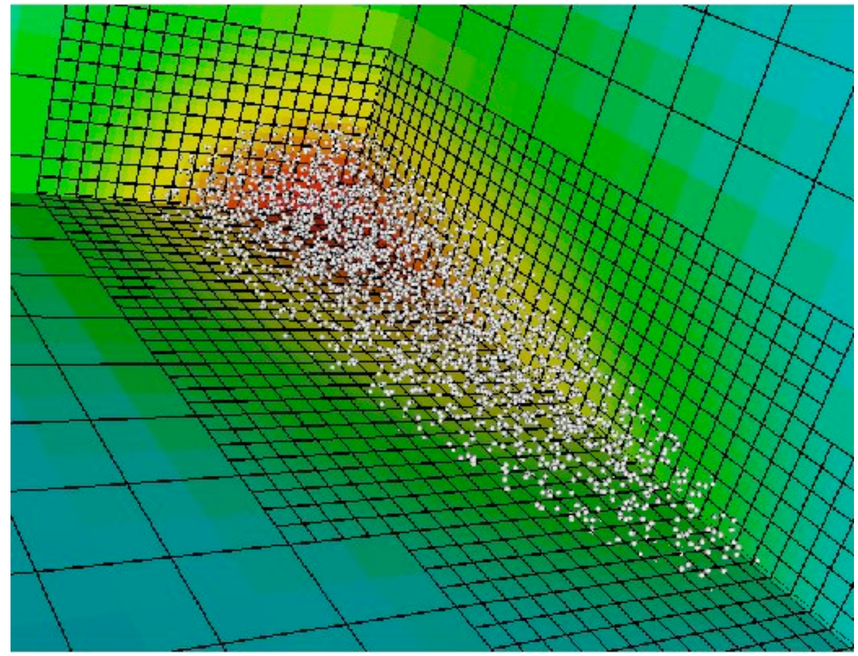


- **WARP is test PIC code but library will be usable by any PIC code**

Examples of pre-AMR-PIC simulations using Chombo



WARP-Chombo injector field calculation*



MLI-Chombo beam field calculation

* P. McCorquodale, P. Colella, D.P. Grote, J.-L. Vay, JCP (2004)

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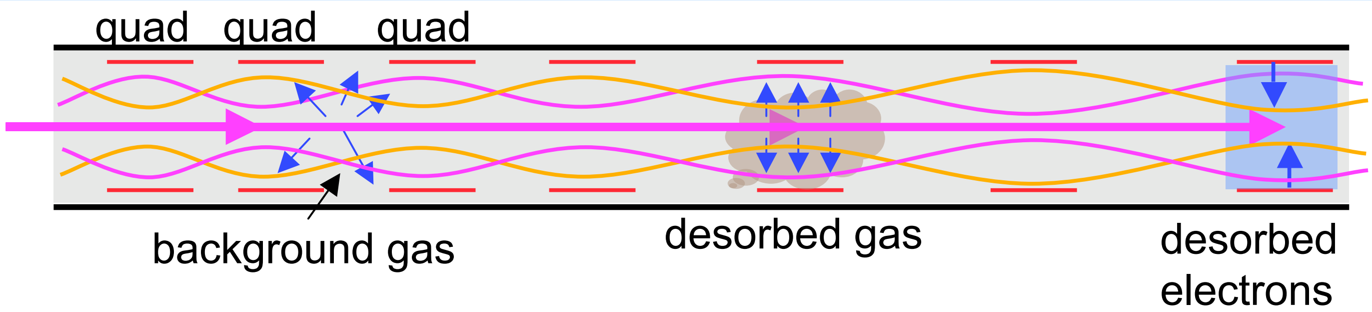
Motivation



- Our historical motivation: e-clouds in induction accelerators for HIF
  - Need to follow electron orbits both in magnets (strongly magnetized) and in between (unmagnetized).
  - Analytic integration of orbits in B field impossible because beam potential known only numerically and can't be considered as impulsive.
- Need a way to accurately calculate electron orbits without having to take timesteps small compared to cyclotron period
- Note:
  - above considerations apply to:
    - other kinds of accelerators
    - plasmas with both strong and weak magnetic fields

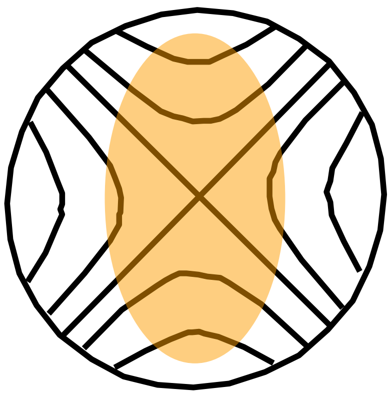
      Magnetic-fusion

      Inertial confinement fusion

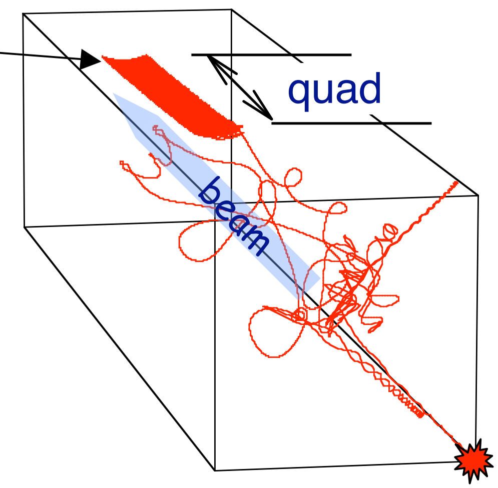
      Space plasmas

Statement of the problem

Magnetic quadrupole



Sample electron motion in a quad



Problem: Electron gyro timescale

<< other timescales of interest

⇒ brute-force integration <u>very</u> slow due to small Δt

- Historical inspiration: Parker & Birdsall (JCP '91)
  - showed that standard Boris mover at large $\omega_c \Delta t$ produces correct ExB and magnetic drifts
  - Price: anomalously large "gyro" radius ($\sim \rho\ \omega_c \Delta t$) and anomalously low "gyro" frequency (particle orbit advances by almost π in gyrophase per timestep; precesses at frequency $\sim 1/\ \omega_c \Delta t^{2}$)
  - For our applications, low "gyro" freq. OK but large "gyroradius" is not

We have developed an interpolation technique that allows us to skip over electron-cyclotron timescale

- Our solution: interpolation between full-electron dynamics (Boris mover) and drift kinetics (motion along B plus drifts).

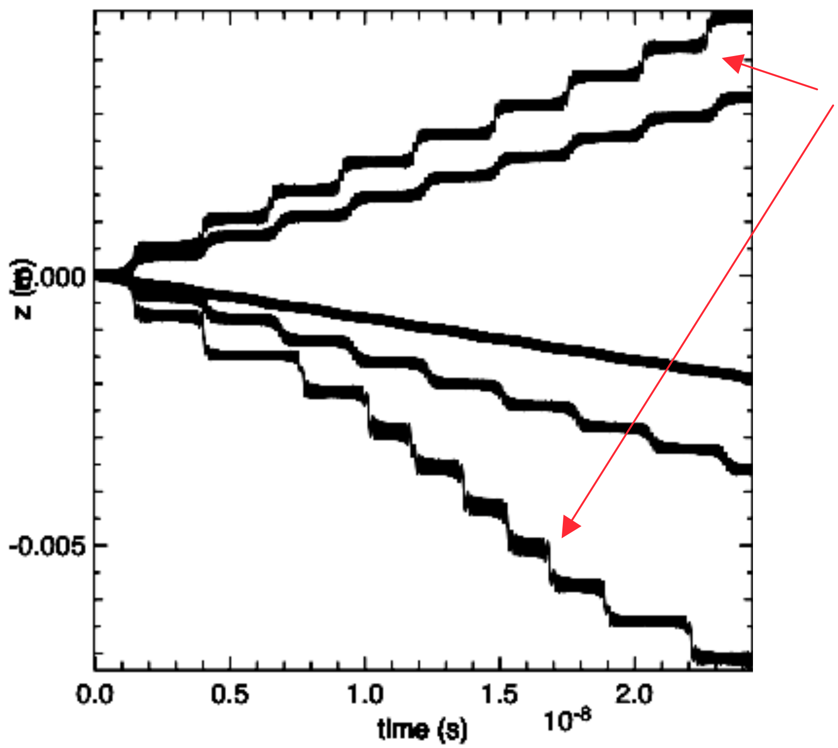
$$\mathbf{v}_{new} = \mathbf{v}_{old} + \Delta t \left(\frac{d\mathbf{v}}{dt}\right)_{Lorentz} + (1-\alpha)\left(\frac{d\mathbf{v}}{dt}\right)_{\mu\nabla B}$$

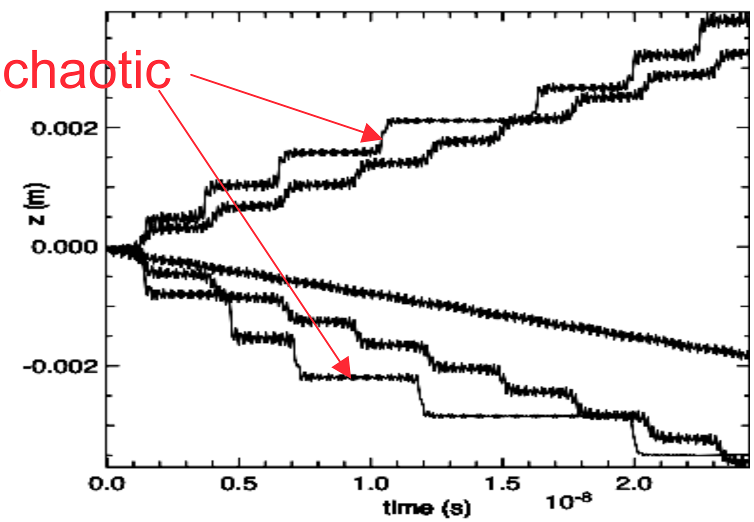
$$\mathbf{v}_{eff} = \mathbf{b}(\mathbf{b}\cdot\mathbf{v}) + \alpha\mathbf{v}_{\perp} + (1-\alpha)\mathbf{v}_d$$

- Choice $\alpha=1/[1+(\omega_c\Delta t/2)^2]^{1/2}$ gives, at both small and large $\omega_c\Delta t$,
  - physically correct “gyro” radius
  - correct drift velocity
  - Correct parallel dynamics.
- Incorrect “gyration frequency” at large $\omega_c\Delta t$ (same as pure Boris mover)
- Time step constraint set by next longer time scale -- typically electron cross-beam transit time.

Test problem: drit orbits in quadrupole field with a specified beam space-charge potential

- Compare full orbit ($\omega_c\Delta t \sim 0.25$) to interpolated mover ($\omega_c\Delta t \sim 2.5$).
- Single orbit comparisons of some regular and nonadiabatic (chaotic) orbits:
  - Chaotic orbits: ones launched on field lines that pass very close to field null.
  - Good agreement on drift & bounce velocity, orbit size for regular orbits
  - Expected non-agreement for chaotic orbits (expect similar statistics, but not tested).

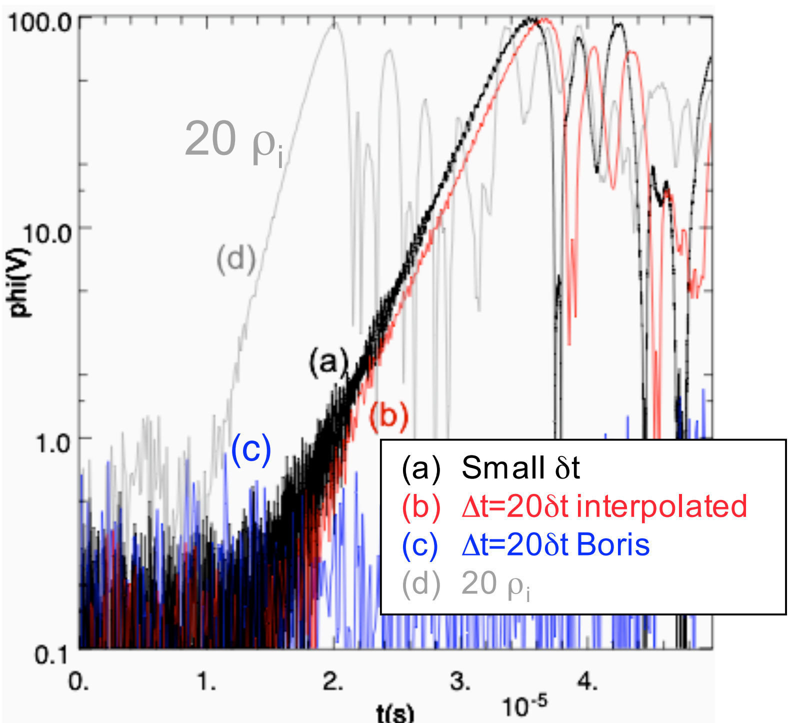




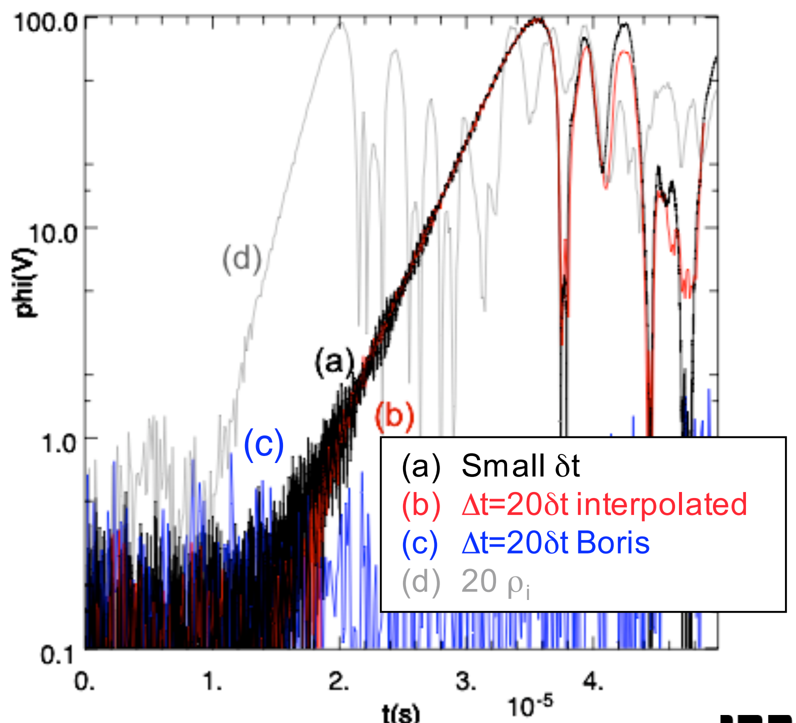
Average slope gives drift, frequency of stairsteps is bounce frequency

Ion-ion two-stream instability test shows good agreement in time histories

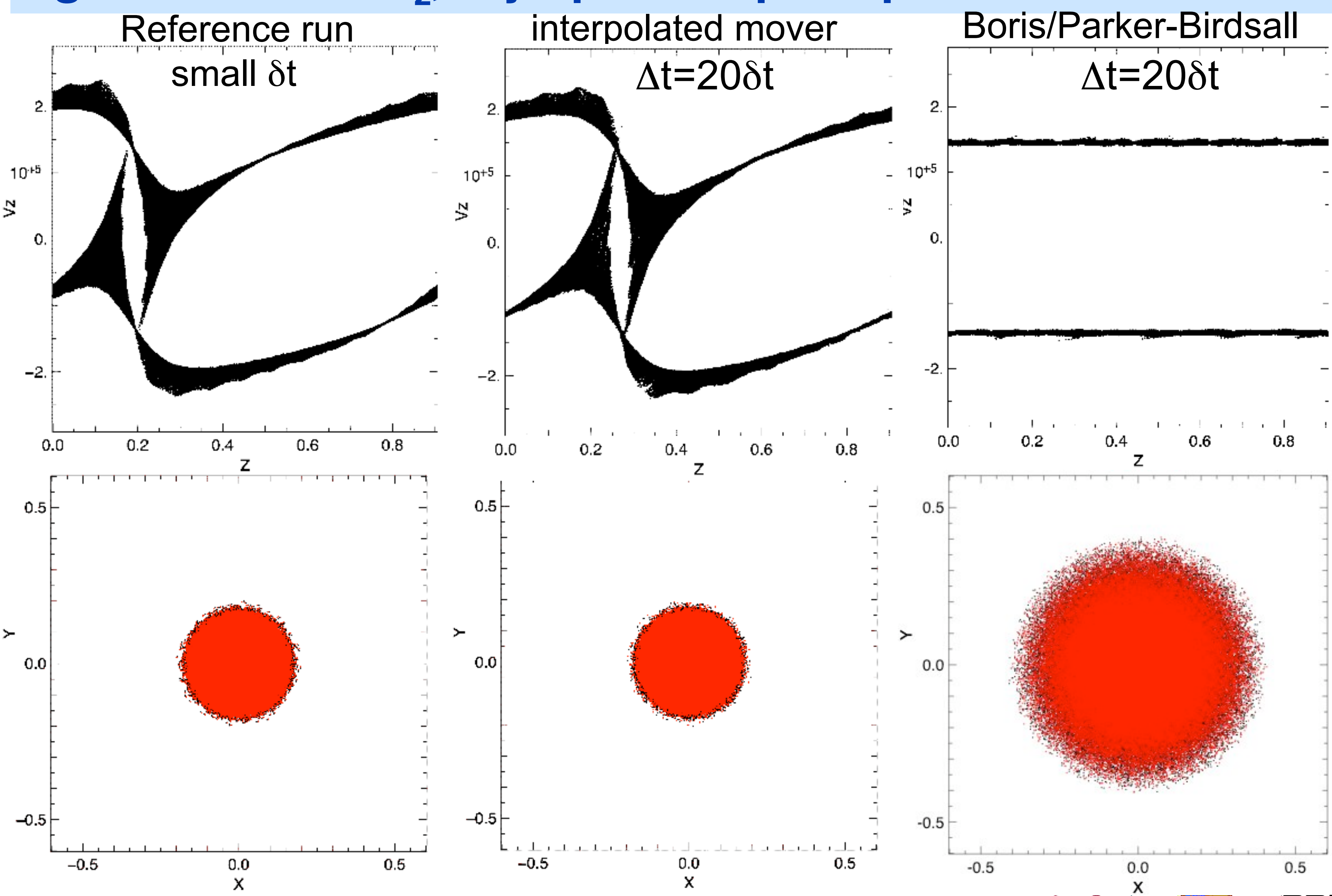
- Test problem:
  - Uniform B field; counter-streaming proton beams along B, 10 ρ_i across
  - $\omega_c/\omega_p = 48$; $v_b/v_{th} = 0.1$; $L/\rho_i \approx 60$
  - Compare: small δt ($\omega_c \delta t = 0.6$), large $\Delta t=20\,\delta t$ ($\omega_c \Delta t = 12$) with interpolation; Δt with Boris mover (Parker-Birdsall)
  - Finite beam-size effect: comparison with 20 ρ_i beam



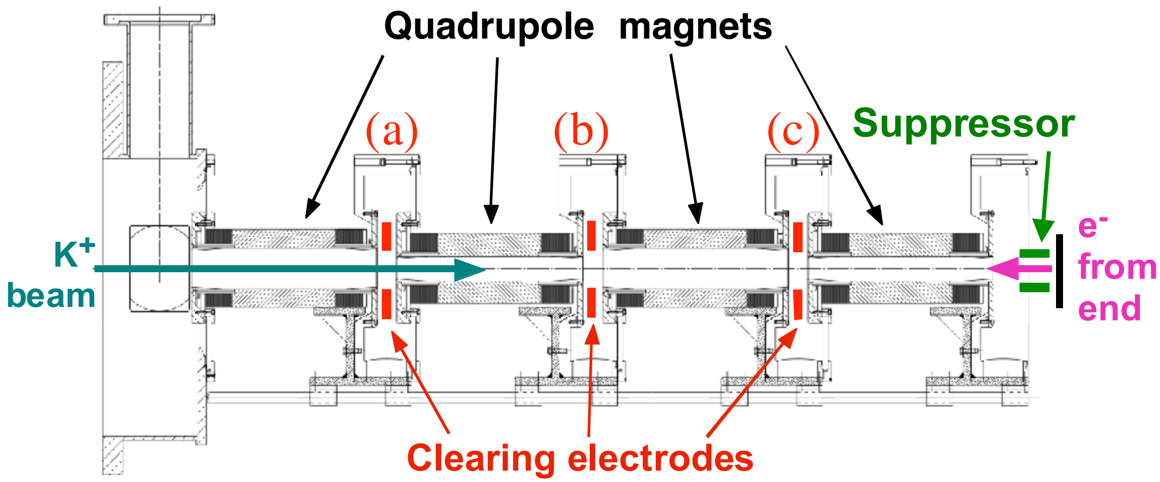
random seed => small time shift of (b)



Ion-ion two-stream instability test shows good agreement in z-v_z, x-y phase space plots

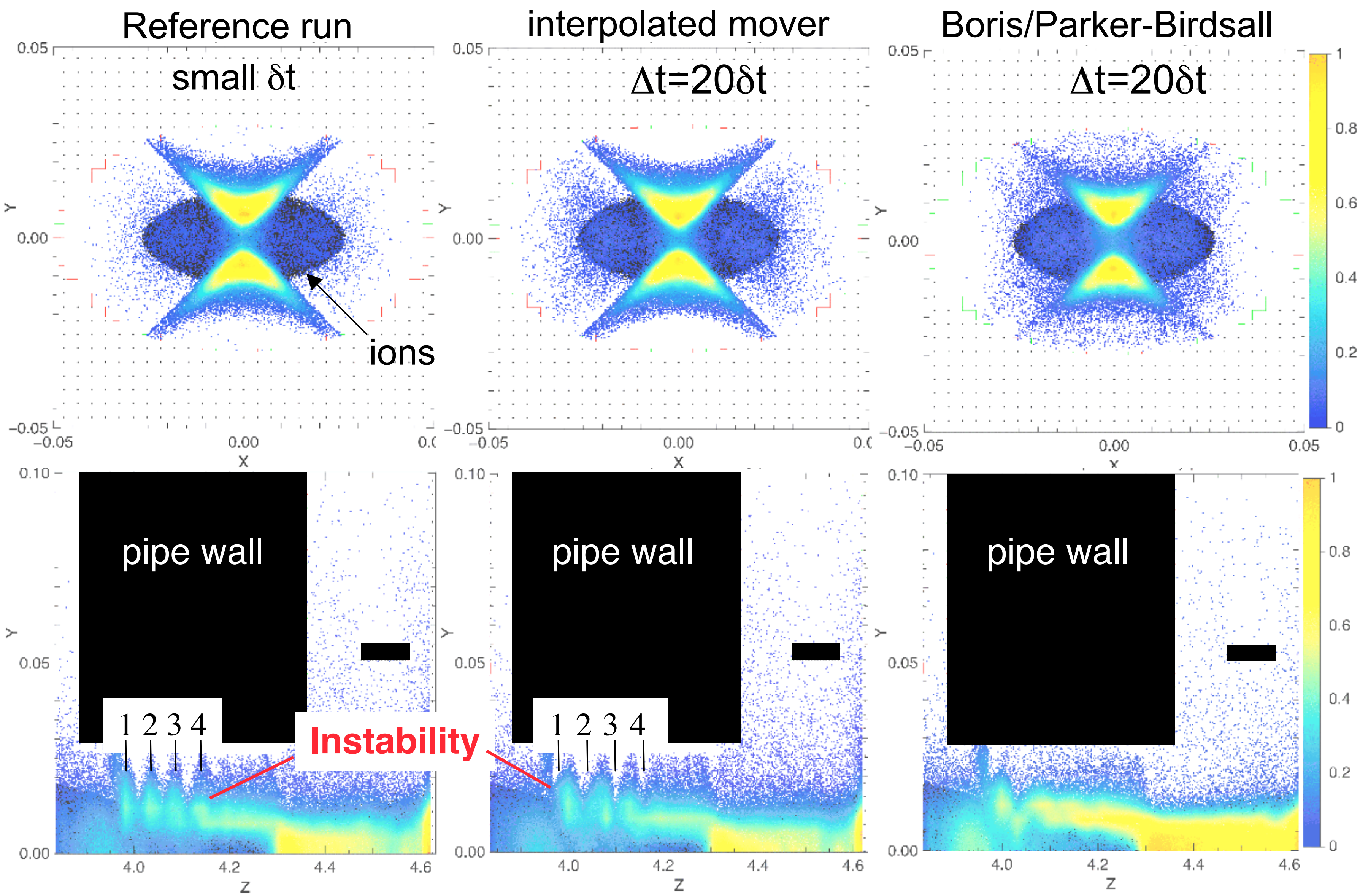


Coupled electron-ion test problem: electrons desorbed at end plate upon ion bombardment



- Simulates experiment performed in High-Current Experiment (HCX) at LBNL
- Ion beam allowed to hit end plate
- Copious electrons produced
- Here: calculate electron cloud produced in fourth magnet
- We have also calculated the electron cloud in all 4 magnets and the resultant change in the ion phase space, and compared with experiment.

Comparison simulations in 4th magnet are another demo that the long-timestep electron mover works



New mover: summary and plans

- Interpolation between Boris algorithm and drift kinetics enables particle simulation with large $\omega_c\Delta t$ that preserves physically correct gyroradius, drifts, and motion parallel to B

- Several tests demonstrate validity of particle mover in situations where simple application of Boris at large $\omega_c\Delta t$ fails.

- Enables simulation on next-longer time scale -- electron bounce motion for the accelerator examples; wave period for the instability example

- Future directions:
  - Bounce orbit averaging or projective integration to jump over electron bounce scales
  - Combine with implicitness and collisions for applications to high-density plasmas

Outline

- Who we are. Our interest in multiscale modeling.
- Modeling of plasmas: generalities.
- AMR
  - issues
  - Electrostatic
    - modeling of the High-Current Experiment (HCX)
    - modeling of the Large Hadron Collider (LHC)
  - Electromagnetic
    - modeling of laser-plasma interaction
  - Vlasov
- New particle mover for large time steps in magnetic fields
- Toward multiscale modeling of plasmas: some methods
- Conclusion

Toward multiscale modeling of plasmas

- A multiscale approach to the modeling of plasmas should
  - advance particles, or group of particles, according to pre-established criteria of accuracy, on an adaptive basis
  - integrate methods that solve on different time scales in one single coherent scheme

- We will look at five methods:
  - Implicit Multiscale PIC (Friedman et al)
  - Discrete Event Simulation PIC (Karimabadi et al)
  - Relaxed Iterative Methods for Coupling Disparate Scales (Shestakov et al)
  - Equation Free Projective Integration (Shay et al)
  - Implicit/explicit solvers coupling (Adam et al)

Implicit MultiScale PIC - IMSPIC

- Advance each particle using a timestep that resolves the local field variations (assumed to be at scale of the grid spacing)
- Implicitness to:
  - Afford stability with $\Delta t > \tau_{plasma}$ and $\Delta x > \lambda_{Debye}$

    in *selected* regions of phase space where that physics is deemed unimportant

    … requires judgment on part of user, and/or smart controls
  - afford a time-centered, second-order-accurate scheme
- Particle push is a variant of "d1" scheme, which allows time step adaptivity

$$v_{n+1} = v_n + \Delta t \left[(3/2)a_{n+1} + (1/2)\bar{a}_{n-1}\right]/2$$
$$x_{n+1} = x_n + \Delta t \left[v_n + (\Delta t/2)a_{n+1}\right]$$

where:

$$\bar{a}_{n-1} = (1/2)a_n + (1/2)\bar{a}_{n-2} \qquad \text{(running sums)}$$

- Poisson equation includes an *"implicit susceptibility"* $\chi(x)$

$$\nabla \cdot \left[(1+\chi)\nabla\phi\right] = \rho, \text{with } \chi(x) = \frac{1}{2}\omega_p^2 \Delta t^2.$$

Timestep sizes are all multiples of some smallest "micro" step size; field-solve is done every micro-step

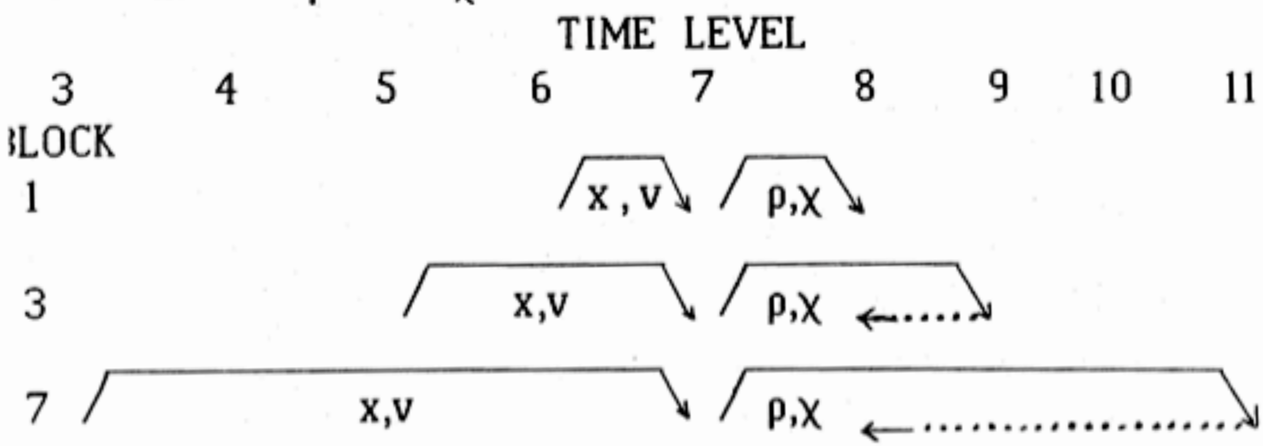
Particles are kept sorted into blocks. For every block k, there is an associated Δt_k; the large timestep used for particles in large cells should help suppress the finite-grid instability. The electron blocks might be:

Block e1: push every step
Block e2: push on even-numbered steps
Block e3: push on odd-numbered steps
Block e4: push if (step number mod 4) = 0
Block e5: push if (step number mod 4) = 1
Block e6: push if (step number mod 4) = 2
Block e7: push if (step number mod 4) = 3

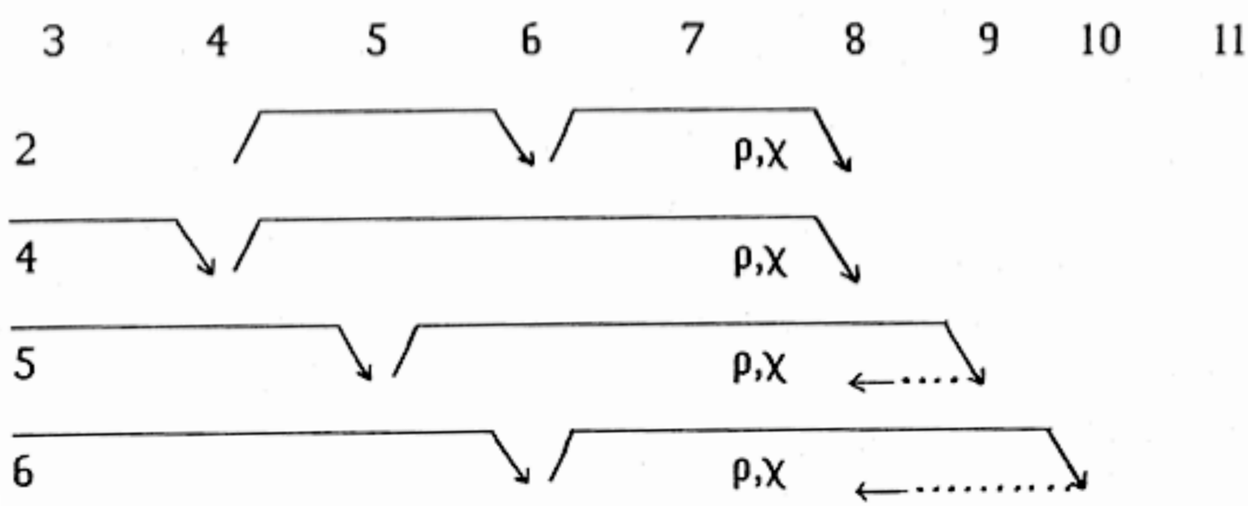
As particles move about, it is necessary to change their Δt's (move them from block to block), in order to preserve the accuracy of their orbits and the deposited charge density.

A timeline shows the procedure for both active and inactive blocks

- Dots with a back-arrow denote interpolation in time of ρ and χ.



The other blocks were advanced on earlier steps, and we need only interpolate their contributions to ρ,χ back to tl 8 before the field-solve:



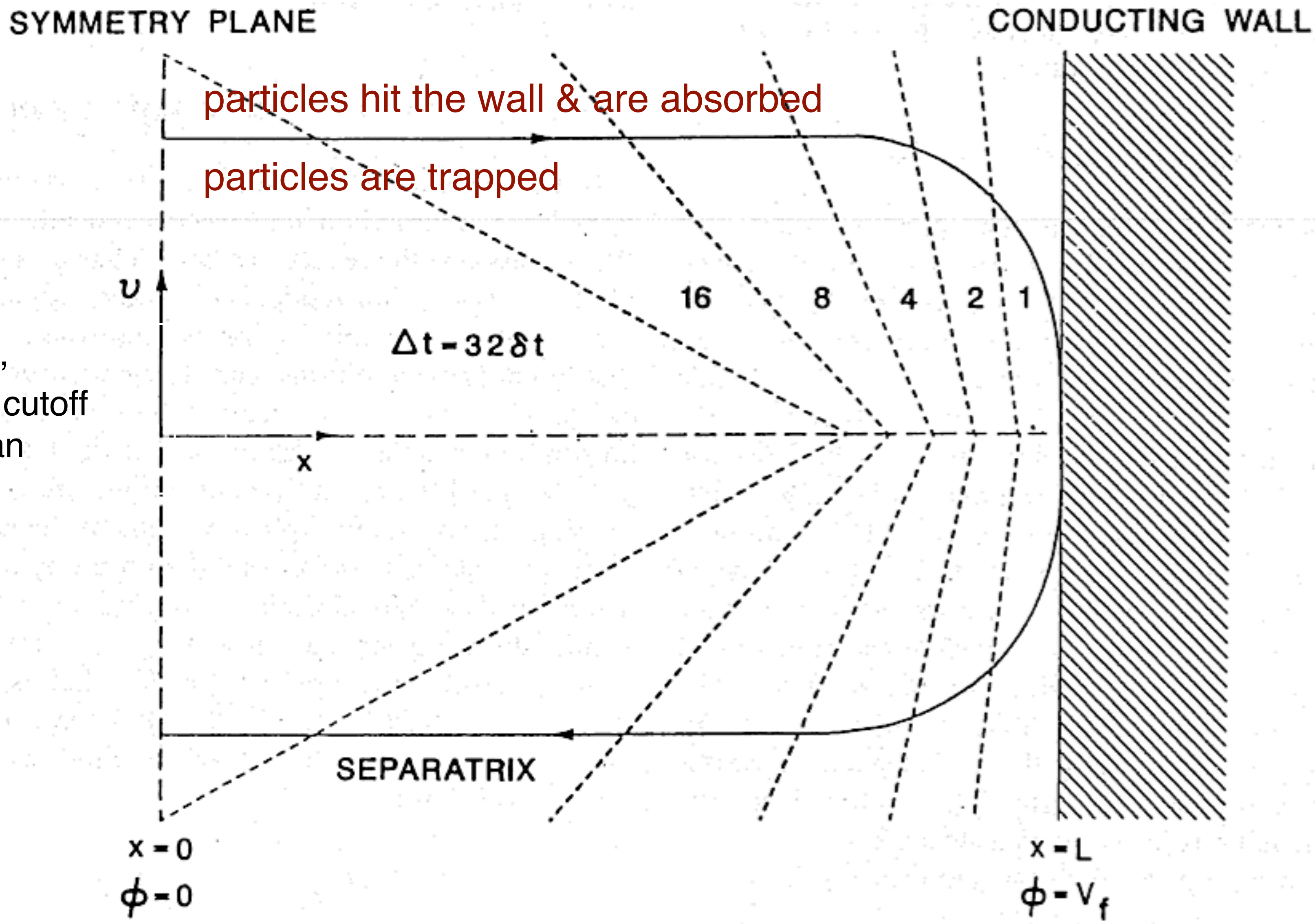
Timestep size control is an "art" as much as a "science"

- Seek to control truncation error
  - Static control associates *ab initio* a step size τ with each location in phase space
  - Dynamic control sets τ based on evolving gradients, etc.

- In the sheath application (see next slides), particle travel through the sheath (∂_xE), rather than the time-dependent variation of E, is most limiting
  - Would like to limit $|kv\Delta t| < \varepsilon_1$, where $k \sim \partial_x E/E$. However, if E and ∂_xE are fluctuating about zero (as is often the case), then where E ~ 0 there may be spuriously large values of k
  - It's somewhat easier to limit $\omega^2_{\mathrm{trap}}\, \Delta t^2 \equiv (q/m)|\partial_x E|\Delta t^2 < \varepsilon_2$ by computing $|\partial_x E|$ on the grid
  - For our sheath work we used static control

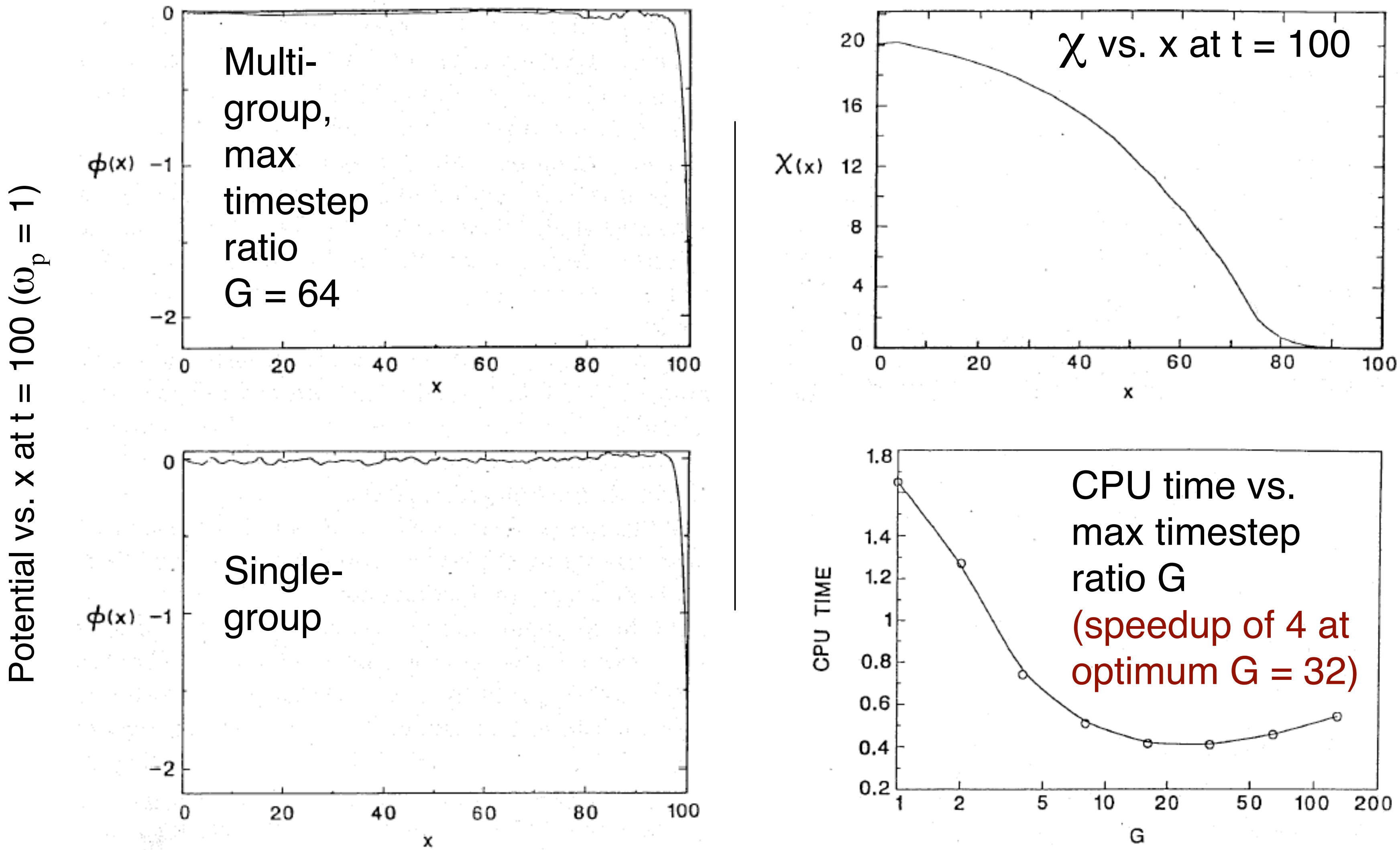
Application to the modeling of a sheath near a “floating” wall

ions fixed,
electrons cutoff
Maxwellian



* S. E. Parker, A. Friedman, S. L. Ray, and C. K. Birdsall, “Bounded Multi-Scale Plasma Simulation: Application to Sheath Problems,” *J. Comp. Phys*. **107**, 388 (1993).

Application to sheath showed effectiveness of method

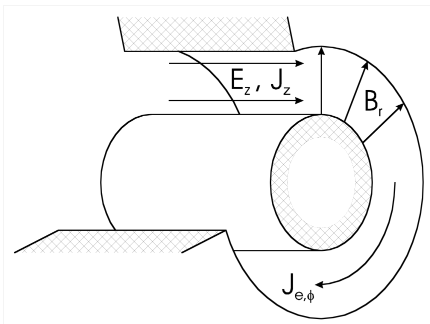


Another series of runs examined propagation of an ion acoustic shock front toward a conducting absorbing plate; see paper by Parker, *et al.*

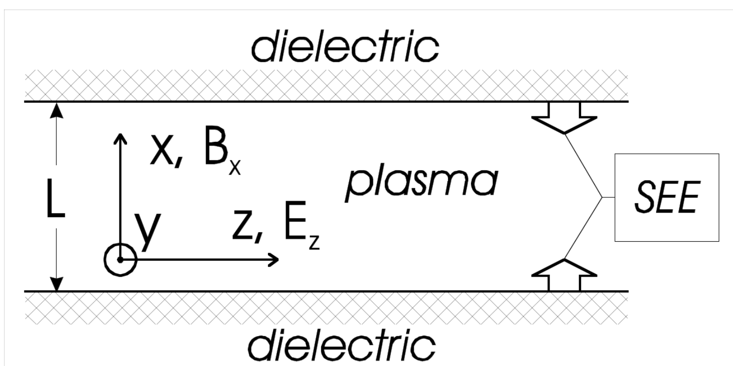
Application of IMSPIC to secondary electron emission (SEE) effects in a plasma slab in crossed electric and magnetic fields

[Sydorenko, Smolyakov, 46th APS DPP, Savannah GA, 2004, NM2B.008]

Hall thruster, cylindrical geometry:



1D3V PIC simulations, plane geometry, approximation of accelerating region of a Hall thruster:



Motivation:

Electron temperature in the accelerating region of a Hall thruster (40 eV) is higher than the temperature of charge saturation of SEE in Maxwellian plasma (17 eV). [Staack, Raitses, Fisch, *Appl. Phys. Lett.* 84, 3028 (2004).]

Objective:

The investigation of modification of electron velocity distribution function by SEE effects.

Simulation requirements:

Both the sheath and the bulk plasma must be resolved.

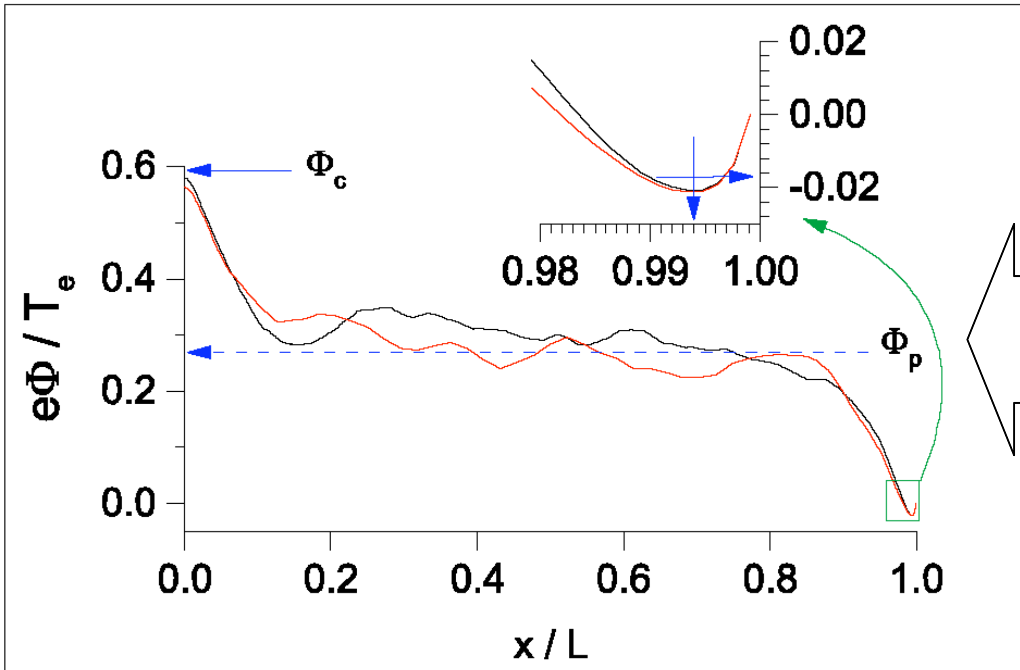
PIC code:

Electrostatic implicit multi-scale with non-uniform grid constant in time. [Friedman, Parker, Ray, Birdsall, *J. Comput. Phys.* 96, 54 (1991).] The external fields B_x and E_z are assumed constant.

Application of IMSPIC to secondary electron emission … Benchmarking of the multi-scale code

The code was applied to simulations of the region between the Maxwellian plasma source (x=0) and the wall with SEE (x=L). No collisions, zero external fields.

Such a problem was considered by Schwager [*Phys. Fluids* B 5, 631 (1993)]



Snapshots of profile of potential.

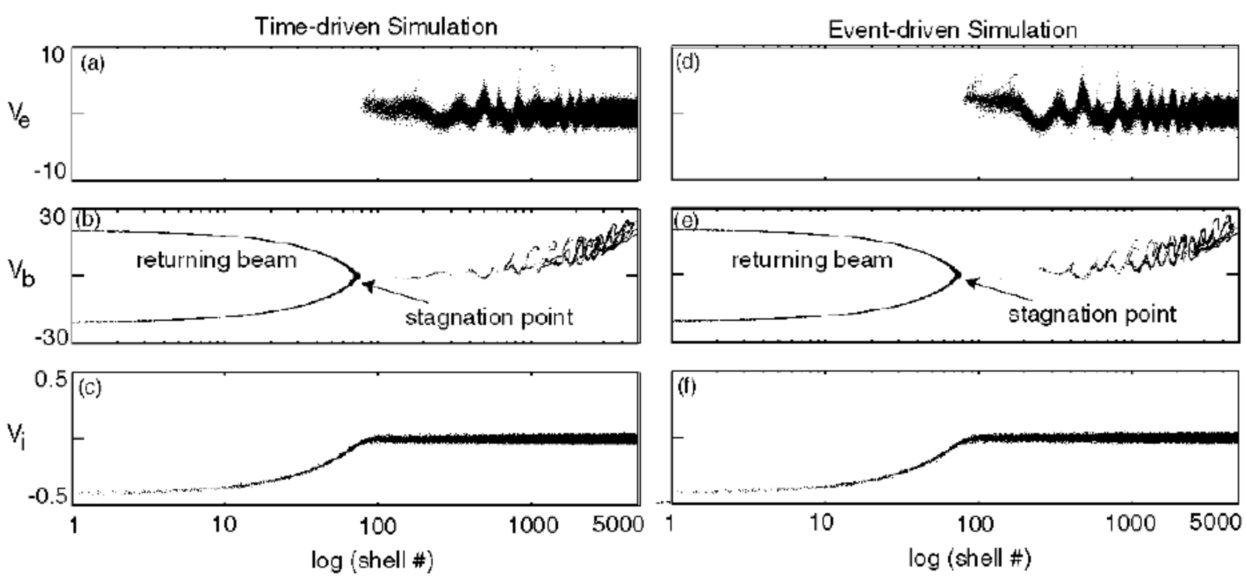
The insert figure zooms into the potential dip near the emitting wall.

- Blue arrows – Schwager's data.
- Black curves – uniform grid,
  $$\Delta x = \lambda_{De}/32, \Delta t = 1/(4\omega_{pe})$$
- Red curves – nonuniform grid,
  $$\Delta x_{\min} = \lambda_{De}/32, \Delta x_{\max}/\Delta x_{\min} = 16;$$
  $$\Delta t_{\min} = 1/(128\omega_{pe}), t_{\max}/\Delta t_{\min} = 64$$

- The results of the single-scale and multi-scale simulations are close to each other and reproduce the results of Schwager.
- The multi-scale simulation is 8 times faster than the single scale simulation.

Discrete Event Simulation is an alternative approach

- DES PIC has similar goals to Implicit Multi-Scale PIC but differs fundamentally
  - Event-driven, not time-driven
  - Particle timesteps fully independent, asynchronous
  - Not (necessarily) implicit
- Builds on established discrete-event methodology
- Incremental field solution may be a challenge
- Successfully applied to spacecraft charging in 1D spherical geometry*:

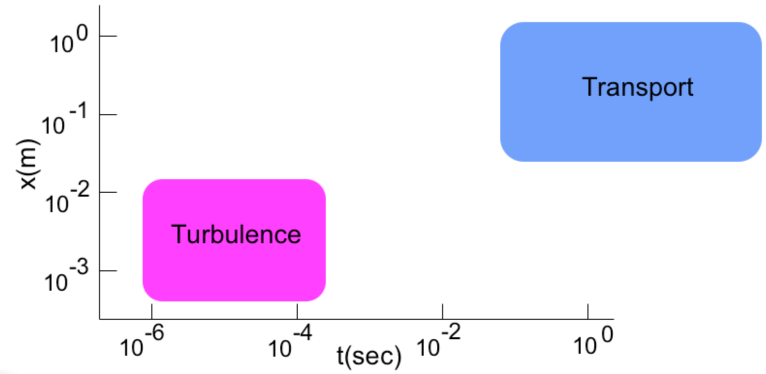


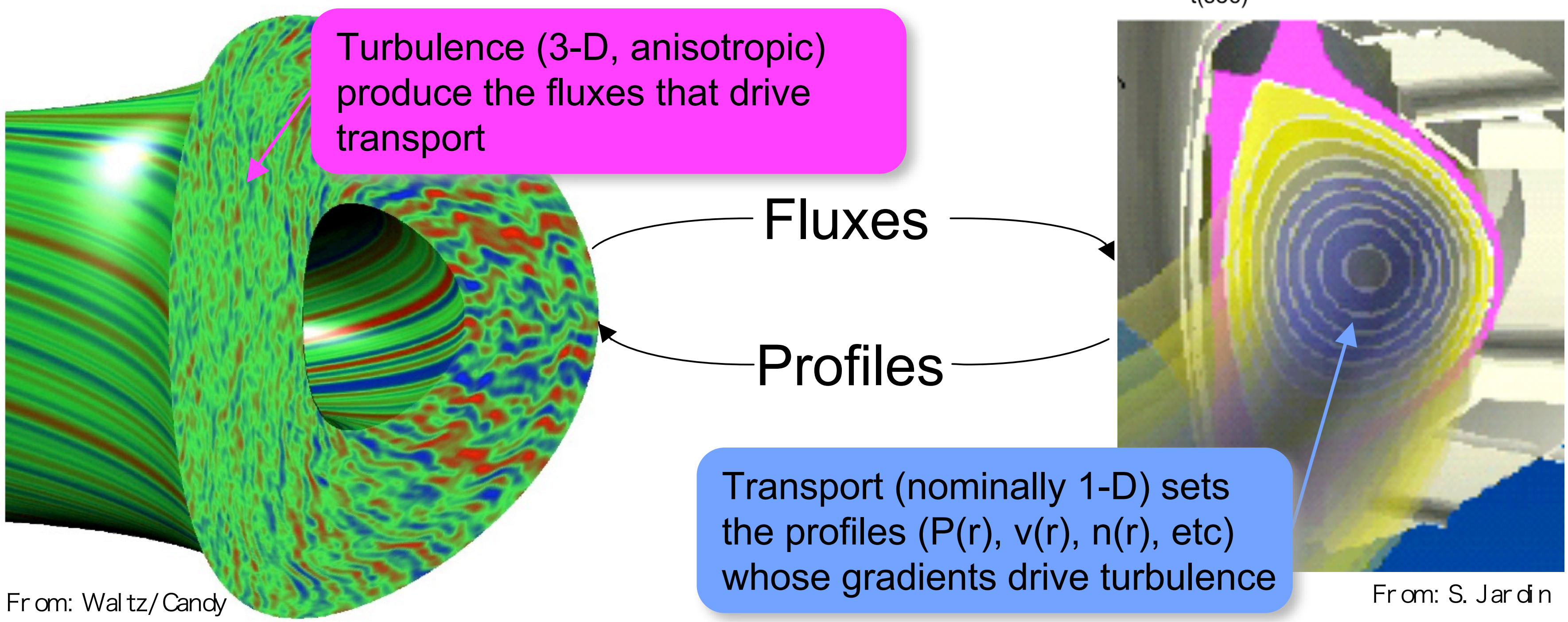
*H. Karimabadi, J. Driscoll, Y. A. Omelchenko, and N. Omidi,to be publ. in *JCP*

Relaxed Iterative Methods for Coupling Disparate Scales (RIC)

Motivation:

- evolution of T, n, v in toroidal MFE devices governed by **transport** which is usually dominated by fluxes driven by plasma **turbulence**
- Significant spread of scales (especially time)





RIC: Step 1, split the equations

- Consider nonlinear equations containing two timescales, of form:

$$\partial_t \mathbf{u} + \nabla \cdot \Gamma(\mathbf{u}) = S,$$

u = density, temperature, etc

- Define average & fluctuating parts $u = \langle u \rangle + \tilde{u}$, $\langle \tilde{u} \rangle = 0$
- Split equations into averaged (transport) and fluctuating (turbulence) parts:

$$\partial_t \langle \mathbf{u} \rangle + \nabla \cdot \langle \Gamma(\mathbf{u}) \rangle = \langle S \rangle, \qquad \text{“transport”}$$

$$\partial_t \tilde{\mathbf{u}} + \nabla \cdot \left[\Gamma(\mathbf{u}) - \langle \Gamma(\mathbf{u}) \rangle \right] = S - \langle S \rangle \qquad \text{“turbulence”}$$

- Notes:
  - $\langle\ \rangle$ denotes average over ensemble, spatial dimension, or time.
  - Method applies to systems where short and long timescales not derivable from single set of eqs.
  - Next step (2) is predicated on disparity of $\langle\ \rangle$ and $\tilde{}$ timescales

RIC: Step 2, solve coupled system via relaxed functional iteration -- fully implicit and Jacobian-free

- δt and Δt = turbulence and transport code timesteps
- **For each iteration j:**

  In the turbulence code:

  - set input profile $\langle \mathbf{u} \rangle = \langle \mathbf{u} \rangle^{n+1,j}$
  - take turb. code timestep
  - $\mathbf{u}^{j+1} \rightarrow \Gamma^{j+1} \rightarrow \langle \Gamma \rangle^{j+1}$

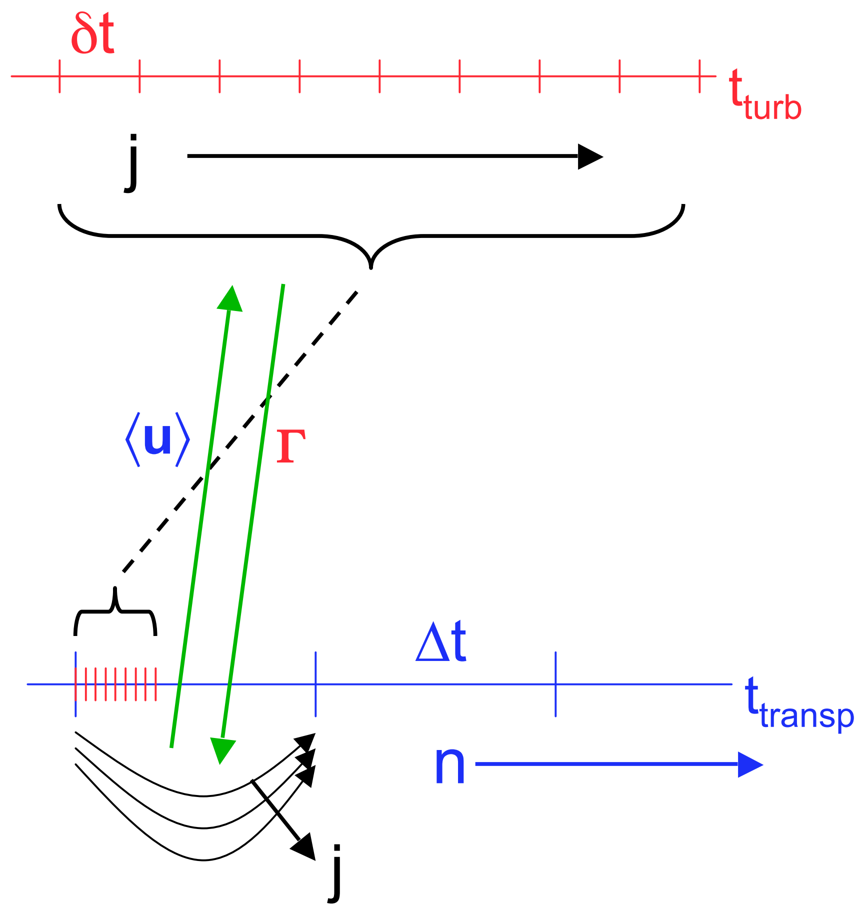
  In the transport code:

  - re-solve the same timestep with updated $\langle \Gamma \rangle^{j+1}$ from turb. code
  - solve as if linear diffusion eqn for $\langle \mathbf{u} \rangle^{n+1,j+1}$ by writing

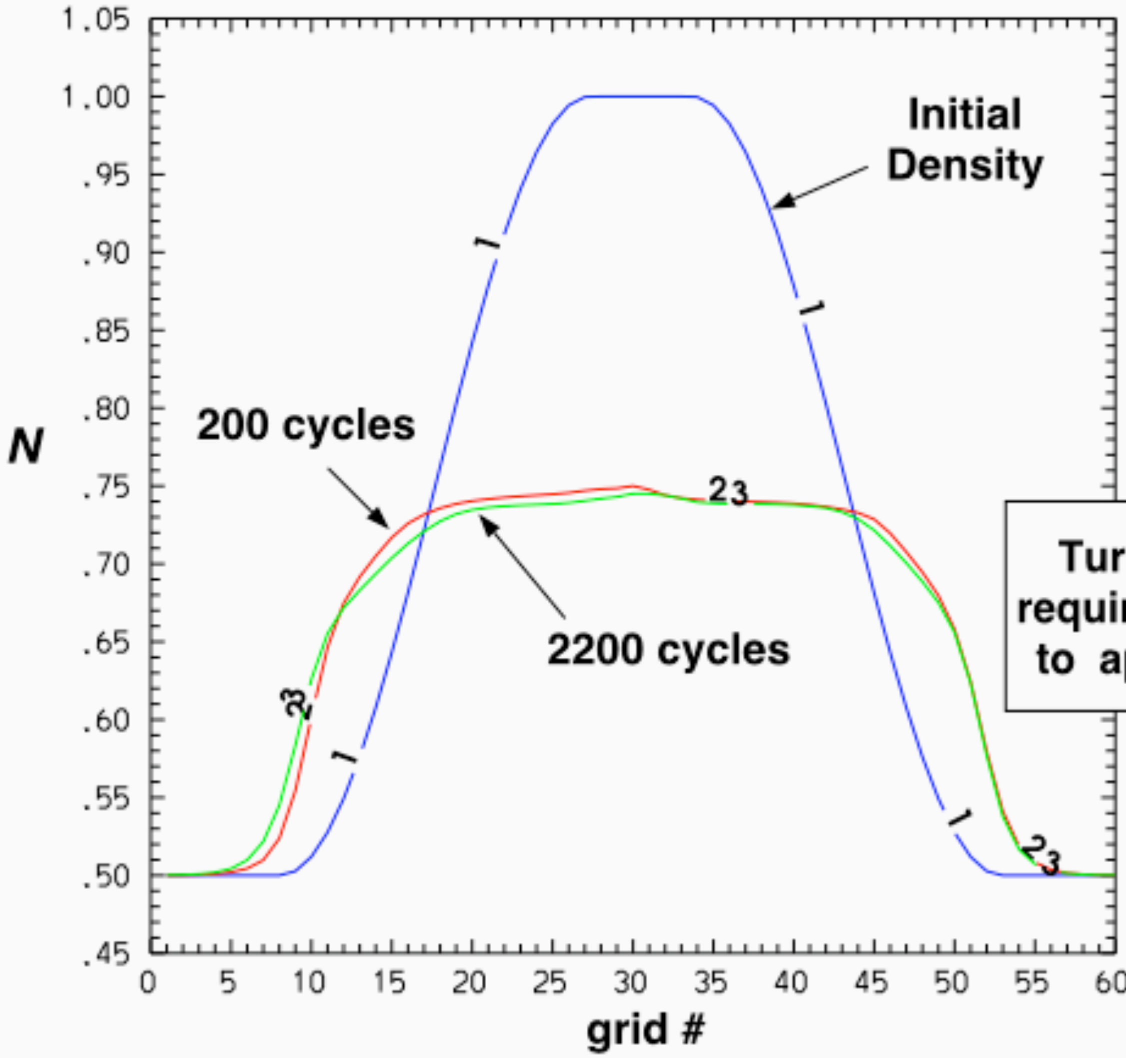
    $\langle \Gamma \rangle = -\mathbf{D} \cdot \nabla \langle \mathbf{u} \rangle^{n+1,j+1}$ with

    $\mathbf{D} = -\overline{\langle \Gamma \rangle}^{j} / \nabla \overline{\langle \mathbf{u} \rangle}^{n+1,j}$

    — denotes relaxed av. over iterates, required for stability.



Coupling simple transport and (HW) turbulence codes achieves rapid relaxation to steady-state transport



Turbulence code alone required > 10,000 timesteps to approach this solution.

RIC summary

- RIC is method which allows running a turbulence code on transport timescale and thus obtain transport profiles self-consistent with turbulent fluxes
- It can be interpreted as an integration of a Delta f and a f solver, which follows both f (transport) and δf (turbulence)
- Fully implicit transport timestepping -- no stability limit on transport timestep
  - one transport timestep (including $\Delta t=\infty$) costs ~ saturated turbulence code run with fixed profiles
  - implies time savings ~ (turbulence timescale/transport timescale)
- A coupling that works for local and (with extensions) non-local transport
  - demonstrated solutions for cases where flux locally runs up-hill

Equation Free Projective Integration

- Projective Integration
  - A method for using a combination of a few small time step integrations to cover large time steps.
- Restriction and Lifting
  - Mappings between a high dimensional representation (microscopic or fine) and a low dimensional representation (macroscopic or coarse), for example:

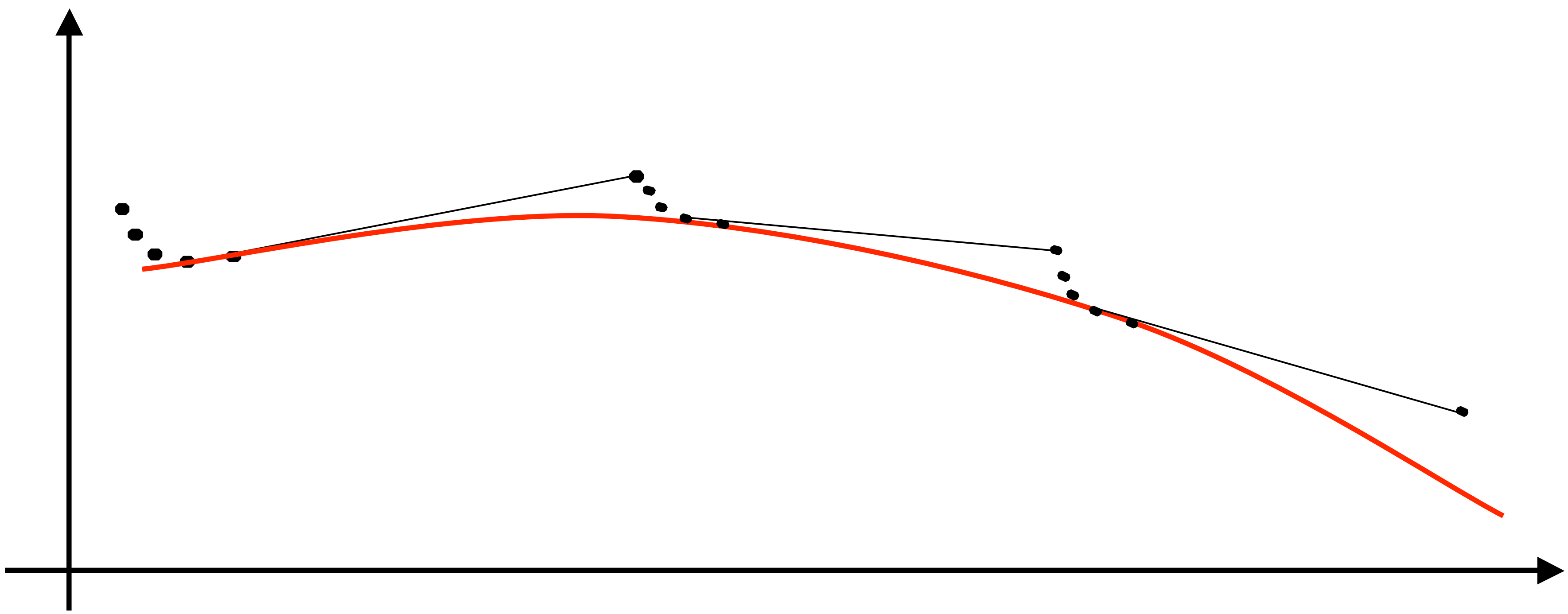
    Microscopic - a collection of particles in Monte Carlo simulations to a low-dimensional description

    Macroscopic - finite element approximation to a *distribution* of the particles
- Projection done on macroscopic representation
- “Experiment” (kinetic code) evaluated on microscopic representation.

Kevrekidis et al., 2002

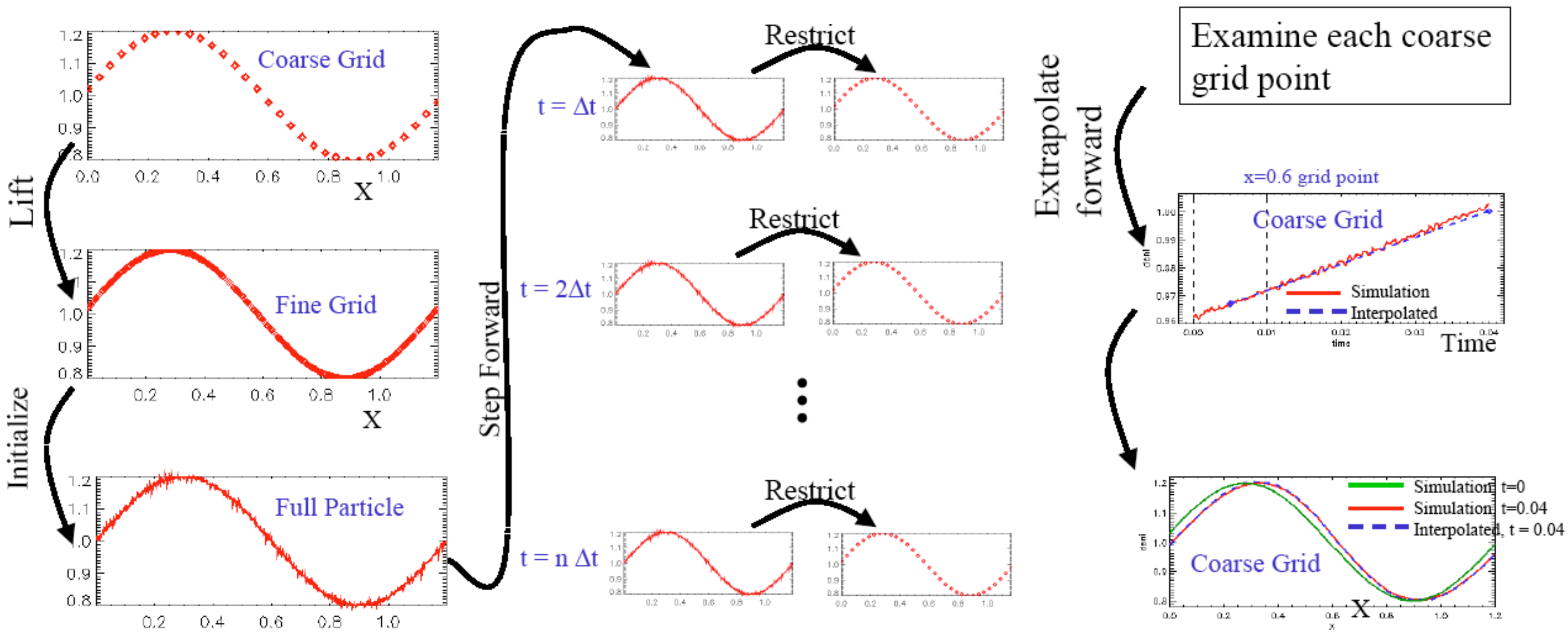
Equation Free Projective Integration

Projective Integration - a sequence of outer integration steps:



Need to study the accuracy and stability of these methods

Equation Free Projective Integration cycle

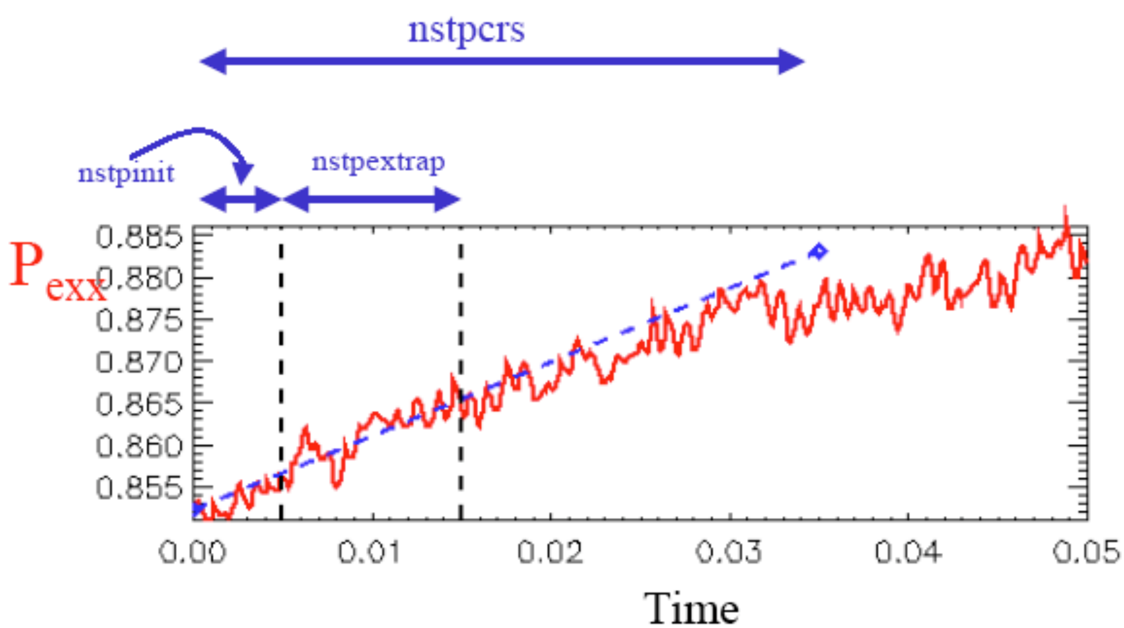


Projecting forward in time

- Use least squares fit.
- Skip nstpinit steps,   fit to nstpextrap steps
- Extrapolate forward nstpcrs steps.
- Use predictor corrector (trapezoidal leapfrog)
  - 2nd order accurate in time

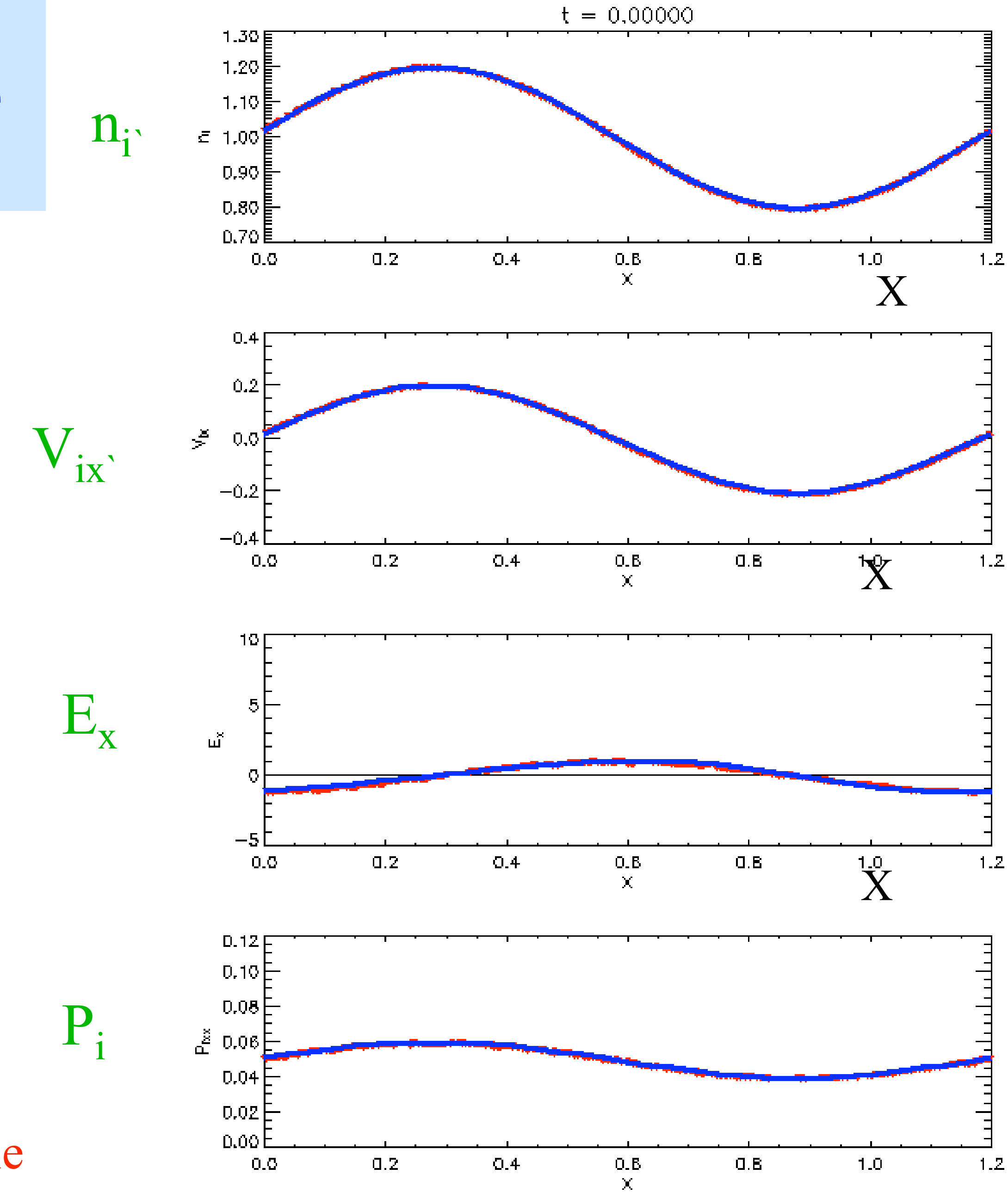
Example

nstpinit = 50
nstpextrap = 100
nstpcrs = 350



Test: ion acoustic mode

- **Wave propagation speed matches exactly.**
- **P_i diverges first.**
- **So far, x12 speed-up**



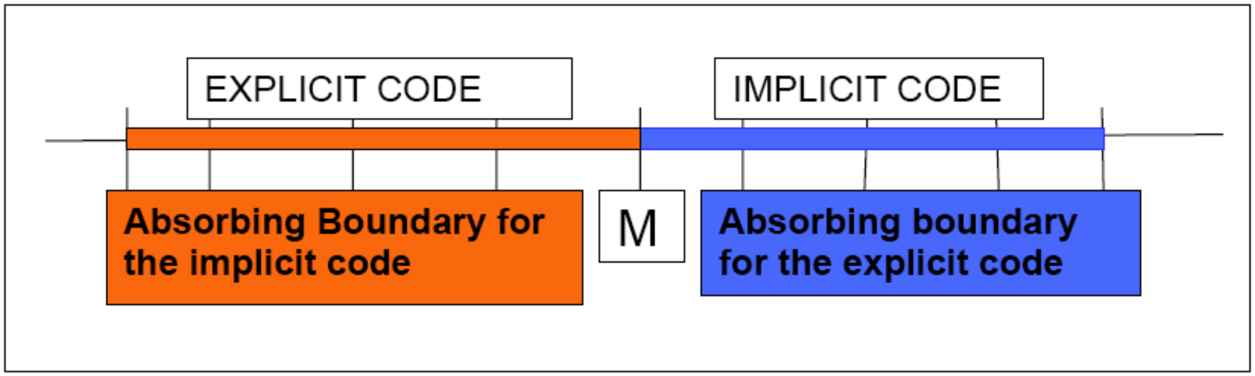
Parameters

$nx_{crs} = 32$
$nx_{micro} = 512$
$lx = 1.2$
$N_{extrap} = 20$
$N_{proj} = 200$

efree
full particle

Coupling of explicit/implicit solvers

- Motivation: high/low density region better handled by implicit/explicit solver.
- J.-C. Adam and A. Héron have proposed to extend the new AMR techniques developed by J.-L. Vay to the coupling of explicit and implicit solvers.



- The left system would be terminated on the right by absorbing boundary conditions that will suppress the outgoing wave of the explicit part, and vice-versa for the right system.
- Particles move freely through the boundary and give the correct source terms in both regions.
- Because mesh size can be different on both sides of the boundary M, mesh refinement is de facto built into the method.

Conclusion

- A lot of effort has been/is devoted to develop techniques to address multiscale issues in plasma modeling.
- AMR can be of great help for PIC/Vlasov multiscale plasma simulations but scheme must be derived with care (spurious self-force, conservation of charge, reflection of waves, non-cancellations due to numerical errors (dispersion), …)
  - in electrostatic, 'problem solved' to some extend but cutoff of plasma modes at interface remains to be studied,
  - in electromagnetic, existing schemes can be successfully applied to some problems but more research is needed to get better scheme(s),
  - with irregular geometries, AMR on regular cartesian grids may not be enough: sometimes need to apply irregularly gridded patch which maps to conductors, field line, …,
- We have developed a new solver that allows to jump over the cyclotron period.
- This is a very active field with several promising emerging methods.

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Equation Free Projective Integration

- http://www.cscamm.umd.edu/cmpd/projective_integration.htm